



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:08 PM UTC

PDB ID : 4BIM / pdb_00004bim
Title : CATALASE 3 FROM NEUROSPORA CRASSA IN TETRAGONAL FORM
EXPOSES A MODIFIED TETRAMERIC ORGANIZATION
Authors : Zarate-Romero, A.; Rudino-Pinera, E.
Deposited on : 2013-04-11
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

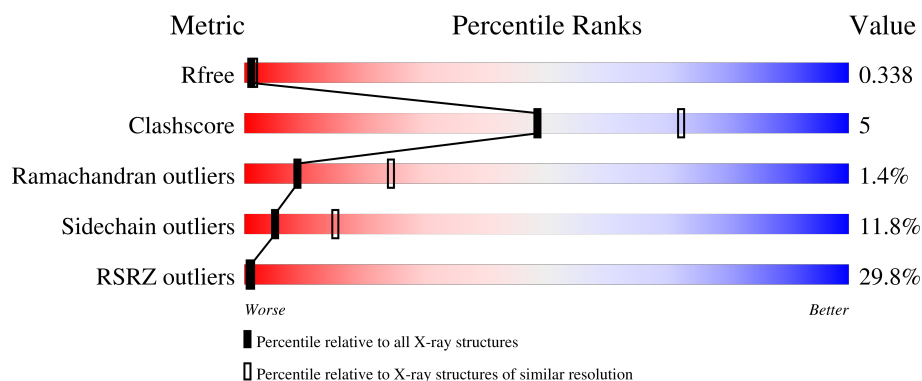
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	746	3% 77% 12% 9%
1	B	746	11% 76% 13% 9%
1	C	746	35% 67% 21% 9%
1	D	746	59% 63% 22% 5% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21809 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CATALASE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	0	0
			5340	3381	941	1012	6			
1	B	679	Total	C	N	O	S	0	0	0
			5324	3371	939	1008	6			
1	C	681	Total	C	N	O	S	0	0	0
			5340	3381	941	1012	6			
1	D	680	Total	C	N	O	S	0	0	0
			5331	3376	940	1009	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP Q9C169
A	-25	ASN	-	expression tag	UNP Q9C169
A	-24	HIS	-	expression tag	UNP Q9C169
A	-23	LYS	-	expression tag	UNP Q9C169
A	-22	VAL	-	expression tag	UNP Q9C169
A	-21	HIS	-	expression tag	UNP Q9C169
A	-20	HIS	-	expression tag	UNP Q9C169
A	-19	HIS	-	expression tag	UNP Q9C169
A	-18	HIS	-	expression tag	UNP Q9C169
A	-17	HIS	-	expression tag	UNP Q9C169
A	-16	HIS	-	expression tag	UNP Q9C169
A	-15	ILE	-	expression tag	UNP Q9C169
A	-14	GLU	-	expression tag	UNP Q9C169
A	-13	GLY	-	expression tag	UNP Q9C169
A	-12	ARG	-	expression tag	UNP Q9C169
A	-11	HIS	-	expression tag	UNP Q9C169
A	-10	MET	-	expression tag	UNP Q9C169
A	-9	GLU	-	expression tag	UNP Q9C169
A	-8	LEU	-	expression tag	UNP Q9C169
A	-7	GLY	-	expression tag	UNP Q9C169
A	-6	THR	-	expression tag	UNP Q9C169

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP Q9C169
A	-4	GLU	-	expression tag	UNP Q9C169
A	-3	GLY	-	expression tag	UNP Q9C169
A	-2	SER	-	expression tag	UNP Q9C169
A	-1	GLU	-	expression tag	UNP Q9C169
A	0	PHE	-	expression tag	UNP Q9C169
B	-26	MET	-	expression tag	UNP Q9C169
B	-25	ASN	-	expression tag	UNP Q9C169
B	-24	HIS	-	expression tag	UNP Q9C169
B	-23	LYS	-	expression tag	UNP Q9C169
B	-22	VAL	-	expression tag	UNP Q9C169
B	-21	HIS	-	expression tag	UNP Q9C169
B	-20	HIS	-	expression tag	UNP Q9C169
B	-19	HIS	-	expression tag	UNP Q9C169
B	-18	HIS	-	expression tag	UNP Q9C169
B	-17	HIS	-	expression tag	UNP Q9C169
B	-16	HIS	-	expression tag	UNP Q9C169
B	-15	ILE	-	expression tag	UNP Q9C169
B	-14	GLU	-	expression tag	UNP Q9C169
B	-13	GLY	-	expression tag	UNP Q9C169
B	-12	ARG	-	expression tag	UNP Q9C169
B	-11	HIS	-	expression tag	UNP Q9C169
B	-10	MET	-	expression tag	UNP Q9C169
B	-9	GLU	-	expression tag	UNP Q9C169
B	-8	LEU	-	expression tag	UNP Q9C169
B	-7	GLY	-	expression tag	UNP Q9C169
B	-6	THR	-	expression tag	UNP Q9C169
B	-5	LEU	-	expression tag	UNP Q9C169
B	-4	GLU	-	expression tag	UNP Q9C169
B	-3	GLY	-	expression tag	UNP Q9C169
B	-2	SER	-	expression tag	UNP Q9C169
B	-1	GLU	-	expression tag	UNP Q9C169
B	0	PHE	-	expression tag	UNP Q9C169
C	-26	MET	-	expression tag	UNP Q9C169
C	-25	ASN	-	expression tag	UNP Q9C169
C	-24	HIS	-	expression tag	UNP Q9C169
C	-23	LYS	-	expression tag	UNP Q9C169
C	-22	VAL	-	expression tag	UNP Q9C169
C	-21	HIS	-	expression tag	UNP Q9C169
C	-20	HIS	-	expression tag	UNP Q9C169
C	-19	HIS	-	expression tag	UNP Q9C169
C	-18	HIS	-	expression tag	UNP Q9C169

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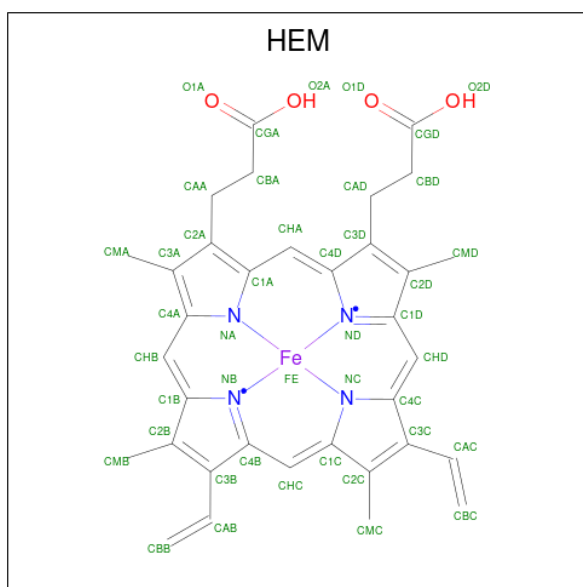
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP Q9C169
C	-16	HIS	-	expression tag	UNP Q9C169
C	-15	ILE	-	expression tag	UNP Q9C169
C	-14	GLU	-	expression tag	UNP Q9C169
C	-13	GLY	-	expression tag	UNP Q9C169
C	-12	ARG	-	expression tag	UNP Q9C169
C	-11	HIS	-	expression tag	UNP Q9C169
C	-10	MET	-	expression tag	UNP Q9C169
C	-9	GLU	-	expression tag	UNP Q9C169
C	-8	LEU	-	expression tag	UNP Q9C169
C	-7	GLY	-	expression tag	UNP Q9C169
C	-6	THR	-	expression tag	UNP Q9C169
C	-5	LEU	-	expression tag	UNP Q9C169
C	-4	GLU	-	expression tag	UNP Q9C169
C	-3	GLY	-	expression tag	UNP Q9C169
C	-2	SER	-	expression tag	UNP Q9C169
C	-1	GLU	-	expression tag	UNP Q9C169
C	0	PHE	-	expression tag	UNP Q9C169
D	-26	MET	-	expression tag	UNP Q9C169
D	-25	ASN	-	expression tag	UNP Q9C169
D	-24	HIS	-	expression tag	UNP Q9C169
D	-23	LYS	-	expression tag	UNP Q9C169
D	-22	VAL	-	expression tag	UNP Q9C169
D	-21	HIS	-	expression tag	UNP Q9C169
D	-20	HIS	-	expression tag	UNP Q9C169
D	-19	HIS	-	expression tag	UNP Q9C169
D	-18	HIS	-	expression tag	UNP Q9C169
D	-17	HIS	-	expression tag	UNP Q9C169
D	-16	HIS	-	expression tag	UNP Q9C169
D	-15	ILE	-	expression tag	UNP Q9C169
D	-14	GLU	-	expression tag	UNP Q9C169
D	-13	GLY	-	expression tag	UNP Q9C169
D	-12	ARG	-	expression tag	UNP Q9C169
D	-11	HIS	-	expression tag	UNP Q9C169
D	-10	MET	-	expression tag	UNP Q9C169
D	-9	GLU	-	expression tag	UNP Q9C169
D	-8	LEU	-	expression tag	UNP Q9C169
D	-7	GLY	-	expression tag	UNP Q9C169
D	-6	THR	-	expression tag	UNP Q9C169
D	-5	LEU	-	expression tag	UNP Q9C169
D	-4	GLU	-	expression tag	UNP Q9C169
D	-3	GLY	-	expression tag	UNP Q9C169

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP Q9C169
D	-1	GLU	-	expression tag	UNP Q9C169
D	0	PHE	-	expression tag	UNP Q9C169

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	61	Total	O	0	0
			61	61		
3	C	54	Total	O	0	0
			54	54		

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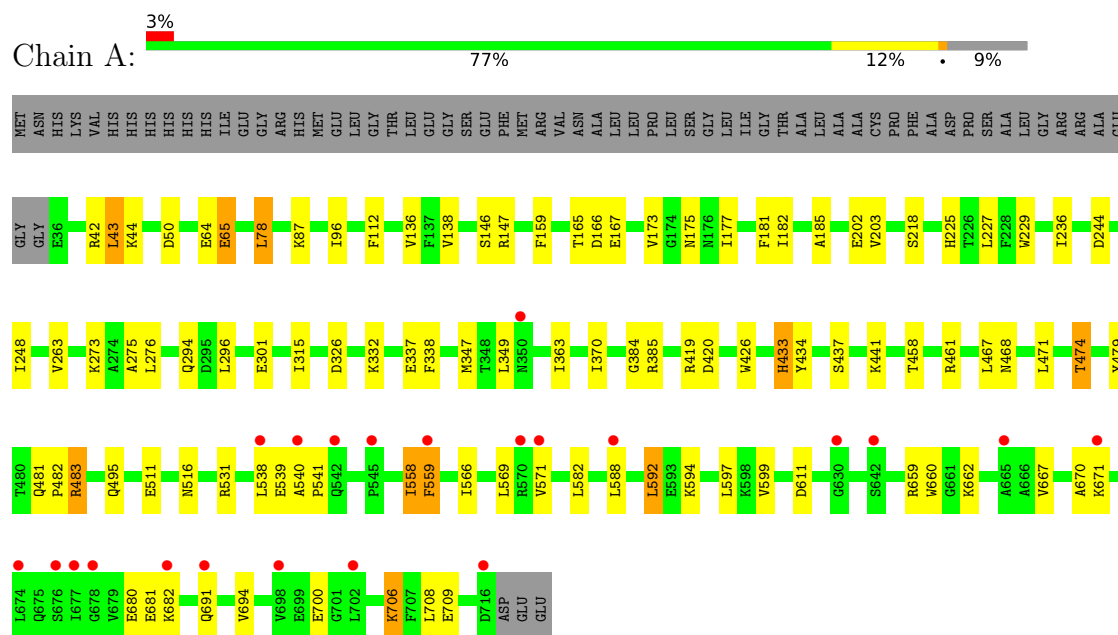
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total	O	0	0
			97	97		

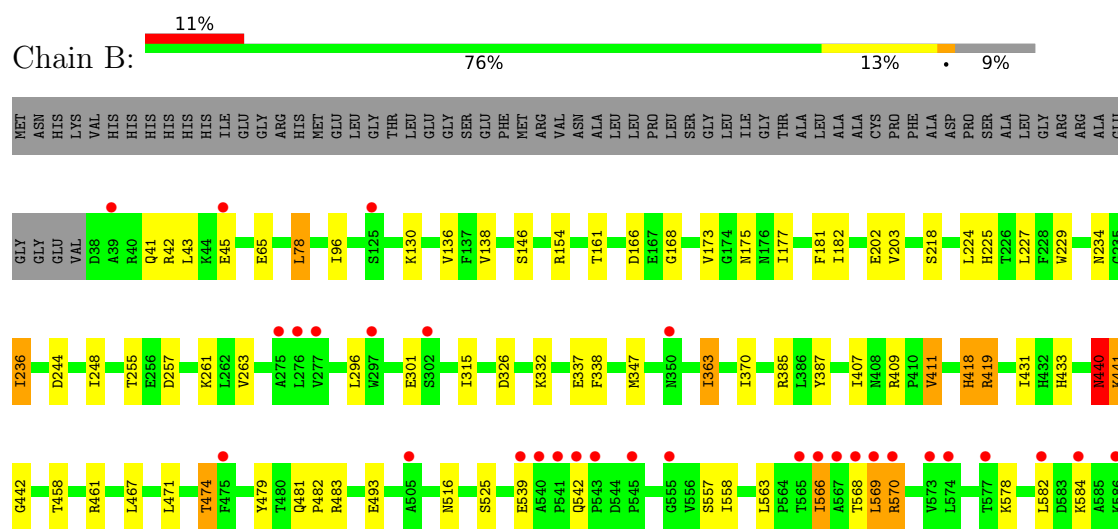
3 Residue-property plots [i](#)

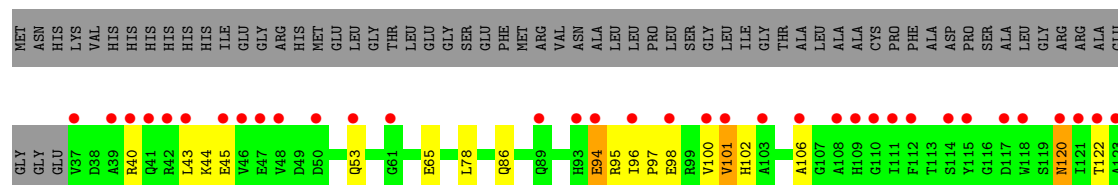
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

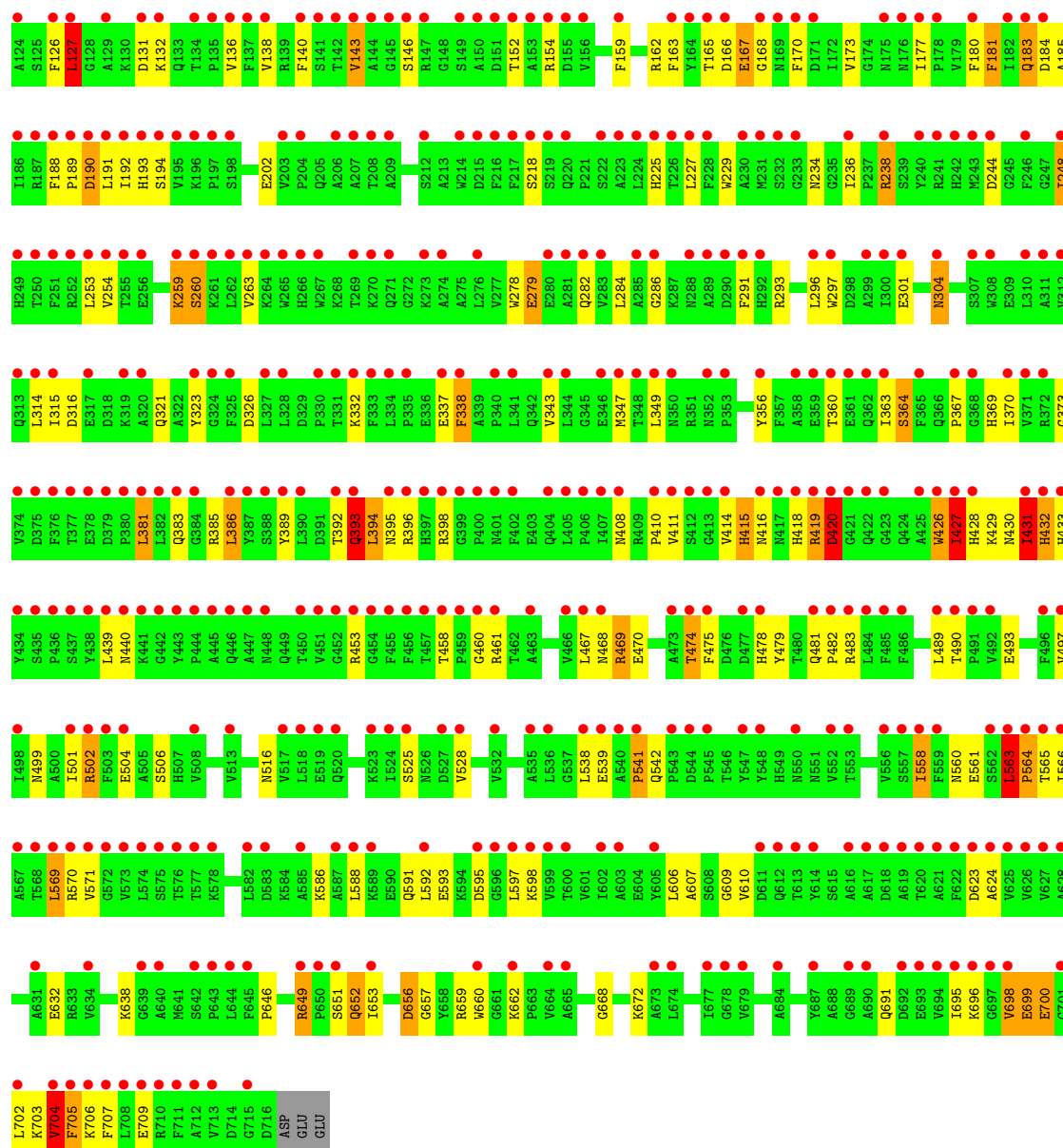
• Molecule 1: CATALASE 3



• Molecule 1: CATALASE 3







4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.51Å 207.51Å 137.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.30 – 2.95 29.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.30-2.95) 98.8 (29.30-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.255 , 0.304 0.285 , 0.338	Depositor DCC
R_{free} test set	3166 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	21809	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.80	1/5473 (0.0%)	1.28	13/7424 (0.2%)
1	B	0.80	0/5457	1.29	18/7402 (0.2%)
1	C	0.83	0/5473	1.37	23/7424 (0.3%)
1	D	0.86	0/5464	1.39	40/7412 (0.5%)
All	All	0.82	1/21867 (0.0%)	1.33	94/29662 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	VAL	CA-C	5.85	1.56	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	541	PRO	CA-C-N	10.52	140.63	121.70
1	C	541	PRO	C-N-CA	10.52	140.63	121.70
1	B	632	GLU	CA-C-N	8.85	137.63	121.70
1	B	632	GLU	C-N-CA	8.85	137.63	121.70
1	C	702	LEU	CA-C-N	8.12	136.31	121.70
1	C	702	LEU	C-N-CA	8.12	136.31	121.70
1	D	304	ASN	CA-CB-CG	7.91	120.51	112.60
1	C	160	ALA	N-CA-C	7.56	120.62	111.40
1	D	420	ASP	CA-CB-CG	7.49	120.09	112.60
1	C	39	ALA	CA-C-N	7.46	135.13	121.70
1	C	39	ALA	C-N-CA	7.46	135.13	121.70
1	C	150	ALA	CA-C-N	7.39	134.99	121.70
1	C	150	ALA	C-N-CA	7.39	134.99	121.70
1	D	698	VAL	CA-C-N	7.27	134.79	121.70
1	D	698	VAL	C-N-CA	7.27	134.79	121.70
1	D	609	GLY	CA-C-N	7.13	134.53	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	609	GLY	C-N-CA	7.13	134.53	121.70
1	D	190	ASP	CA-CB-CG	7.08	119.69	112.60
1	B	566	ILE	CA-C-N	7.07	134.43	121.70
1	B	566	ILE	C-N-CA	7.07	134.43	121.70
1	C	646	PRO	N-CA-C	6.84	122.53	113.57
1	B	338	PHE	CA-CB-CG	6.69	120.49	113.80
1	D	704	VAL	CA-C-N	6.68	133.72	121.70
1	D	704	VAL	C-N-CA	6.68	133.72	121.70
1	D	190	ASP	CA-C-N	6.54	129.57	120.29
1	D	190	ASP	C-N-CA	6.54	129.57	120.29
1	A	338	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	50	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	426	TRP	CA-C-N	6.10	132.69	121.70
1	D	426	TRP	C-N-CA	6.10	132.69	121.70
1	C	84	PHE	CA-C-N	6.06	128.40	120.28
1	C	84	PHE	C-N-CA	6.06	128.40	120.28
1	C	159	PHE	CA-CB-CG	6.03	119.83	113.80
1	D	497	VAL	CA-C-N	5.96	128.19	120.56
1	D	497	VAL	C-N-CA	5.96	128.19	120.56
1	A	541	PRO	CA-C-N	5.95	132.40	121.70
1	A	541	PRO	C-N-CA	5.95	132.40	121.70
1	D	181	PHE	CA-CB-CG	5.83	119.62	113.80
1	D	338	PHE	CA-CB-CG	5.77	119.57	113.80
1	B	411	VAL	CA-C-N	5.76	129.07	120.31
1	B	411	VAL	C-N-CA	5.76	129.07	120.31
1	B	668	GLY	CA-C-N	5.74	129.86	120.63
1	B	668	GLY	C-N-CA	5.74	129.86	120.63
1	D	189	PRO	CA-C-N	5.72	128.22	120.38
1	D	189	PRO	C-N-CA	5.72	128.22	120.38
1	C	338	PHE	CA-CB-CG	5.71	119.51	113.80
1	D	393	GLN	N-CA-C	5.70	118.27	111.71
1	D	501	ILE	CA-C-N	5.70	128.19	120.38
1	D	501	ILE	C-N-CA	5.70	128.19	120.38
1	C	91	PHE	N-CA-C	-5.66	105.48	112.90
1	C	41	GLN	N-CA-C	-5.64	107.64	114.75
1	D	468	ASN	CA-C-N	5.64	131.86	121.70
1	D	468	ASN	C-N-CA	5.64	131.86	121.70
1	C	698	VAL	N-CA-C	-5.63	104.86	111.00
1	D	558	ILE	CA-C-N	5.56	129.50	120.60
1	D	558	ILE	C-N-CA	5.56	129.50	120.60
1	D	102	HIS	CA-C-N	5.52	127.68	120.28
1	D	102	HIS	C-N-CA	5.52	127.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	364	SER	CA-C-N	5.49	129.56	120.94
1	D	364	SER	C-N-CA	5.49	129.56	120.94
1	B	181	PHE	CA-CB-CG	5.46	119.27	113.80
1	B	168	GLY	N-CA-C	5.46	117.61	112.04
1	D	704	VAL	N-CA-CB	5.42	120.17	111.23
1	C	468	ASN	N-CA-C	5.41	117.28	109.07
1	B	440	ASN	CA-CB-CG	5.38	117.98	112.60
1	B	387	TYR	CA-C-N	5.36	127.77	120.54
1	B	387	TYR	C-N-CA	5.36	127.77	120.54
1	B	409	ARG	N-CA-C	5.35	117.19	109.48
1	D	414	VAL	N-CA-C	5.32	115.56	108.11
1	A	159	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	194	SER	N-CA-C	-5.27	104.45	112.04
1	A	540	ALA	N-CA-C	5.25	119.99	108.66
1	B	78	LEU	CA-C-N	5.24	127.83	120.28
1	B	78	LEU	C-N-CA	5.24	127.83	120.28
1	A	559	PHE	N-CA-C	5.21	119.62	113.16
1	C	141	SER	N-CA-C	5.17	115.37	108.38
1	A	181	PHE	CA-CB-CG	5.15	118.95	113.80
1	A	426	TRP	N-CA-C	5.14	117.94	109.72
1	D	656	ASP	N-CA-C	-5.12	101.41	109.25
1	C	224	LEU	N-CA-C	5.11	117.74	111.82
1	D	408	ASN	CA-C-N	5.10	130.17	121.35
1	D	408	ASN	C-N-CA	5.10	130.17	121.35
1	B	224	LEU	N-CA-C	5.09	117.72	111.82
1	A	166	ASP	N-CA-C	-5.06	107.26	112.93
1	C	177	ILE	N-CA-CB	-5.05	106.21	111.61
1	D	143	VAL	CA-C-N	5.04	127.97	120.31
1	D	143	VAL	C-N-CA	5.04	127.97	120.31
1	A	468	ASN	N-CA-C	5.03	116.84	109.24
1	D	120	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	78	LEU	CA-C-N	5.01	127.50	120.28
1	A	78	LEU	C-N-CA	5.01	127.50	120.28
1	D	420	ASP	N-CA-C	5.01	121.47	110.80
1	C	280	GLU	CA-C-N	5.00	127.23	120.38
1	C	280	GLU	C-N-CA	5.00	127.23	120.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5340	0	5156	34	0
1	B	5324	0	5141	34	0
1	C	5340	0	5156	86	0
1	D	5331	0	5151	92	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	90	0	0	1	0
3	B	61	0	0	1	0
3	C	54	0	0	0	0
3	D	97	0	0	2	1
All	All	21809	0	20724	230	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (230) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:704:VAL:HA	1:D:705:PHE:HB3	1.17	1.13
1:C:153:ALA:HB1	1:C:154:ARG:HA	1.22	1.10
1:D:415:HIS:HB2	1:D:416:ASN:HA	1.34	1.09
1:C:102:HIS:HA	1:C:142:THR:O	1.69	0.92
1:D:431:ILE:HD13	1:D:432:HIS:H	1.35	0.91
1:C:646:PRO:HB3	1:D:279:GLU:HG2	1.63	0.79
1:C:39:ALA:HB1	1:C:351:ARG:HG3	1.64	0.79
1:D:152:THR:HG21	1:D:284:LEU:HG	1.67	0.76
1:D:704:VAL:CA	1:D:705:PHE:HB3	2.09	0.75
1:C:153:ALA:HB1	1:C:154:ARG:CA	2.13	0.73
1:D:699:GLU:HG3	1:D:700:GLU:HG2	1.75	0.69
1:B:655:THR:O	1:B:659:ARG:HG2	1.93	0.68
1:C:654:LEU:HB3	1:C:674:LEU:HD13	1.74	0.68
1:D:426:TRP:HA	1:D:427:ILE:HB	1.75	0.68
1:C:287:LYS:HE2	1:D:282:GLN:HG3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLU:HB3	1:C:580:GLY:HA3	1.77	0.67
1:C:104:ARG:HE	1:C:151:ASP:HB2	1.58	0.67
1:C:158:GLY:HA2	1:C:175:ASN:HA	1.77	0.67
1:C:91:PHE:O	1:C:94:GLU:HB2	1.95	0.67
1:C:332:LYS:HG2	1:C:481:GLN:HG3	1.76	0.66
1:D:180:PHE:HB2	1:D:248:ILE:HD13	1.78	0.65
1:C:646:PRO:HG3	1:C:649:ARG:HE	1.62	0.65
1:D:138:VAL:HG11	1:D:349:LEU:HD11	1.78	0.65
1:D:385:ARG:HG2	1:D:389:TYR:HE1	1.62	0.65
1:A:248:ILE:HD13	2:A:4000:HEM:HMB1	1.80	0.64
1:D:238:ARG:HH22	1:D:291:PHE:HZ	1.44	0.64
1:C:278:TRP:H	1:C:496:PHE:HE1	1.45	0.64
1:D:431:ILE:CD1	1:D:432:HIS:H	2.10	0.64
1:A:483:ARG:NH2	3:A:2070:HOH:O	2.30	0.63
1:D:260:SER:HB3	1:D:458:THR:HG21	1.80	0.63
1:D:563:LEU:HB3	1:D:564:PRO:HA	1.80	0.63
1:D:704:VAL:HA	1:D:705:PHE:CB	2.08	0.63
1:A:571:VAL:HG11	1:A:592:LEU:HD22	1.81	0.62
1:C:625:VAL:HB	1:C:654:LEU:HD12	1.81	0.62
1:C:606:LEU:HD21	1:D:506:SER:HB2	1.80	0.62
1:D:563:LEU:H	1:D:703:LYS:HG2	1.64	0.62
1:C:248:ILE:HD13	2:C:4000:HEM:HMB1	1.82	0.61
1:B:248:ILE:HD13	2:B:4000:HEM:HMB1	1.82	0.61
1:C:417:ASN:HB3	1:C:433:HIS:O	2.01	0.61
1:D:419:ARG:HE	1:D:420:ASP:HB3	1.66	0.60
1:C:40:ARG:HD2	1:C:43:LEU:HD12	1.82	0.60
1:C:540:ALA:HB1	1:C:541:PRO:CD	2.32	0.60
1:D:668:GLY:HA3	3:D:2064:HOH:O	2.02	0.59
1:C:153:ALA:CB	1:C:154:ARG:HA	2.12	0.58
1:C:93:HIS:ND1	1:D:395:ASN:HB2	2.18	0.58
1:B:569:LEU:HD13	1:B:598:LYS:H	1.68	0.58
1:D:154:ARG:HH12	1:D:504:GLU:HG3	1.69	0.58
1:C:702:LEU:HD12	1:C:705:PHE:HA	1.84	0.58
1:D:415:HIS:HB2	1:D:416:ASN:CA	2.23	0.57
1:C:57:THR:HG23	1:C:63:ILE:HG12	1.86	0.57
1:D:571:VAL:HG22	1:D:624:ALA:HB3	1.84	0.57
1:D:563:LEU:HB3	1:D:564:PRO:CA	2.34	0.57
1:D:183:GLN:HG2	1:D:475:PHE:HD2	1.69	0.57
1:C:284:LEU:HD13	1:C:620:THR:HB	1.87	0.57
1:C:177:ILE:HG12	1:C:229:TRP:HB3	1.87	0.56
1:D:415:HIS:CB	1:D:416:ASN:HA	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:646:PRO:HD2	1:D:649:ARG:HG3	1.87	0.56
1:D:489:LEU:HB3	1:D:493:GLU:HB3	1.88	0.55
1:A:177:ILE:HG12	1:A:229:TRP:HB3	1.89	0.54
1:D:431:ILE:HD13	1:D:432:HIS:N	2.14	0.54
1:D:385:ARG:HG2	1:D:389:TYR:CE1	2.43	0.54
1:C:483:ARG:HD2	1:C:525:SER:HB2	1.89	0.54
1:B:177:ILE:HG12	1:B:229:TRP:HB3	1.89	0.54
1:C:533:ALA:HB1	1:C:539:GLU:HA	1.90	0.54
1:D:177:ILE:HG12	1:D:229:TRP:HB3	1.90	0.54
1:D:483:ARG:HD2	1:D:525:SER:HB2	1.90	0.54
1:A:136:VAL:HG21	1:A:347:MET:HG3	1.90	0.53
1:B:136:VAL:HG21	1:B:347:MET:HG3	1.90	0.53
1:C:138:VAL:HG22	1:C:161:THR:HG22	1.89	0.53
1:D:180:PHE:CD2	1:D:381:LEU:HD21	2.43	0.53
1:D:165:THR:OG1	1:D:168:GLY:O	2.25	0.53
1:A:275:ALA:HB3	1:A:558:ILE:HD13	1.90	0.53
1:A:467:LEU:HD22	1:B:78:LEU:HD11	1.90	0.53
1:C:632:GLU:HG3	1:C:673:ALA:HB2	1.91	0.52
1:D:136:VAL:HG21	1:D:347:MET:HG3	1.92	0.52
1:D:97:PRO:HD2	1:D:396:ARG:HA	1.91	0.52
1:C:100:VAL:HA	1:D:95:ARG:HG3	1.90	0.52
1:C:39:ALA:CB	1:C:351:ARG:HG3	2.38	0.52
1:C:282:GLN:O	1:D:286:GLY:HA3	2.10	0.52
1:B:483:ARG:HD2	1:B:525:SER:HB2	1.92	0.52
1:C:90:HIS:H	1:C:93:HIS:HD2	1.58	0.52
1:B:660:TRP:HE3	1:B:662:LYS:HE3	1.75	0.51
1:C:635:PHE:CE1	1:C:674:LEU:HD12	2.45	0.51
1:D:185:ALA:HA	2:D:4000:HEM:HBB1	1.92	0.51
1:A:419:ARG:HG3	1:A:433:HIS:HD2	1.76	0.51
1:A:458:THR:HB	1:A:461:ARG:HG3	1.92	0.51
1:A:276:LEU:HA	1:A:706:LYS:HE3	1.92	0.51
1:D:660:TRP:HE3	1:D:662:LYS:HE3	1.76	0.50
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.94	0.50
1:C:156:VAL:HG23	1:C:177:ILE:HD12	1.94	0.50
1:C:102:HIS:CE1	1:C:143:VAL:HG22	2.46	0.50
1:C:574:LEU:HD21	1:C:653:ILE:HG23	1.92	0.50
1:C:589:LYS:O	1:C:593:GLU:HB2	2.10	0.50
1:D:323:TYR:HD1	1:D:338:PHE:CD2	2.29	0.50
1:A:660:TRP:HE3	1:A:662:LYS:HE3	1.76	0.49
1:A:273:LYS:HB3	1:A:558:ILE:HG22	1.93	0.49
1:D:696:LYS:HA	1:D:699:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD11	1:B:467:LEU:HD22	1.94	0.49
1:B:234:ASN:ND2	1:B:558:ILE:HD11	2.27	0.49
1:D:278:TRP:O	1:D:282:GLN:HG2	2.12	0.49
1:A:42:ARG:HG2	1:A:43:LEU:HD22	1.95	0.49
1:B:568:THR:OG1	1:B:569:LEU:HA	2.13	0.49
1:C:136:VAL:HG21	1:C:347:MET:HG3	1.94	0.49
1:B:458:THR:HB	1:B:461:ARG:HG3	1.94	0.48
1:C:325:PHE:HB2	1:C:332:LYS:HD3	1.94	0.48
1:D:418:HIS:CG	1:D:419:ARG:H	2.29	0.48
1:D:699:GLU:HA	1:D:700:GLU:HA	1.65	0.48
1:B:418:HIS:O	1:B:419:ARG:HD3	2.13	0.48
1:C:94:GLU:O	1:C:95:ARG:NH1	2.46	0.48
1:D:383:GLN:O	1:D:386:LEU:HG	2.13	0.48
1:C:366:GLN:HG2	1:C:390:LEU:HD22	1.95	0.48
1:C:566:ILE:HD13	1:C:699:GLU:HG2	1.95	0.48
1:C:458:THR:HB	1:C:461:ARG:HG3	1.94	0.48
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.95	0.48
1:C:39:ALA:HB3	1:C:40:ARG:HB3	1.95	0.48
1:D:234:ASN:ND2	1:D:558:ILE:HD11	2.29	0.48
1:D:364:SER:HB3	1:D:393:GLN:CD	2.39	0.47
1:C:276:LEU:HA	1:C:706:LYS:HE3	1.96	0.47
1:C:606:LEU:HA	1:C:610:VAL:HB	1.97	0.47
1:D:122:THR:HB	1:D:253:LEU:HB3	1.95	0.47
1:C:153:ALA:HB2	1:C:235:GLY:O	2.14	0.47
1:D:652:GLN:NE2	1:D:656:ASP:OD2	2.46	0.47
1:C:39:ALA:HB2	1:C:351:ARG:HH11	1.79	0.47
1:C:518:LEU:HB3	1:C:540:ALA:HB2	1.96	0.47
1:D:260:SER:HB3	1:D:458:THR:CG2	2.45	0.47
1:A:566:ILE:HA	1:A:569:LEU:HD12	1.96	0.47
1:A:495:GLN:OE1	1:A:531:ARG:NH2	2.37	0.47
1:B:708:LEU:HD22	1:B:708:LEU:H	1.79	0.47
1:C:144:ALA:HB3	1:C:155:ASP:OD2	2.15	0.46
1:C:202:GLU:HB2	1:D:356:TYR:CG	2.50	0.46
1:C:225:HIS:CE1	1:C:481:GLN:HB3	2.49	0.46
1:D:323:TYR:HD1	1:D:338:PHE:HD2	1.61	0.46
1:C:637:GLY:O	1:C:641:MET:HB2	2.16	0.46
1:D:254:VAL:N	1:D:373:GLY:O	2.47	0.46
1:B:154:ARG:HG3	1:B:236:ILE:HG23	1.97	0.46
1:B:175:ASN:HB2	1:B:248:ILE:HD11	1.97	0.46
1:C:111:ILE:HD11	1:C:133:GLN:HG2	1.97	0.46
1:C:284:LEU:HD11	1:C:291:PHE:CD1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:LEU:HB2	1:C:597:LEU:HD23	1.96	0.46
1:C:310:LEU:HD23	1:C:344:LEU:HB2	1.98	0.46
1:C:432:HIS:HB2	1:C:440:ASN:HB3	1.96	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.16	0.46
1:C:540:ALA:HB1	1:C:541:PRO:HD3	1.98	0.45
1:D:188:PHE:CZ	1:D:192:ILE:HD11	2.51	0.45
1:C:623:ASP:HB3	1:C:702:LEU:HD11	1.98	0.45
1:A:175:ASN:HB2	1:A:248:ILE:HD11	1.98	0.45
1:D:563:LEU:CB	1:D:564:PRO:HA	2.46	0.45
1:D:106:ALA:HB2	1:D:293:ARG:HG2	1.98	0.45
1:C:143:VAL:HG23	1:C:156:VAL:O	2.17	0.45
1:C:218:SER:HB2	1:C:516:ASN:HB3	1.99	0.45
1:D:623:ASP:O	1:D:662:LYS:HB3	2.16	0.45
1:B:261:LYS:HB2	3:B:2013:HOH:O	2.16	0.45
1:C:116:GLY:HA2	1:C:130:LYS:HG3	1.99	0.45
1:A:165:THR:C	1:A:167:GLU:H	2.25	0.45
1:B:440:ASN:HD22	1:B:442:GLY:H	1.65	0.45
1:C:467:LEU:HD22	1:D:78:LEU:HD11	1.98	0.45
1:A:138:VAL:HG23	1:A:349:LEU:HD21	1.99	0.45
1:A:559:PHE:CD2	1:A:708:LEU:HD21	2.51	0.45
1:D:490:THR:OG1	1:D:493:GLU:HB2	2.17	0.45
1:B:569:LEU:HD22	1:B:597:LEU:HA	1.99	0.44
1:D:314:LEU:HD23	1:D:314:LEU:H	1.82	0.44
1:D:418:HIS:HB3	1:D:430:ASN:HD22	1.82	0.44
1:B:650:PRO:HA	1:B:653:ILE:HD12	1.99	0.44
1:D:564:PRO:HD2	3:D:2026:HOH:O	2.16	0.44
1:A:571:VAL:HG13	1:A:599:VAL:HG13	1.99	0.44
1:C:93:HIS:HE1	1:D:394:LEU:HG	1.83	0.44
1:C:173:VAL:HB	1:C:385:ARG:HH22	1.83	0.44
1:D:569:LEU:O	1:D:623:ASP:HB2	2.17	0.44
1:A:559:PHE:HB3	1:A:708:LEU:HD11	2.00	0.44
1:D:181:PHE:HB2	1:D:191:LEU:HD11	2.00	0.43
1:B:363:ILE:HD12	1:B:407:ILE:HG13	2.00	0.43
1:D:218:SER:HB2	1:D:516:ASN:HB3	2.00	0.43
1:C:336:GLU:H	1:C:336:GLU:HG2	1.59	0.43
1:C:652:GLN:NE2	1:D:652:GLN:OE1	2.52	0.43
1:C:153:ALA:CB	1:C:236:ILE:HG23	2.49	0.43
1:C:479:TYR:C	1:C:482:PRO:HD2	2.44	0.43
1:A:173:VAL:HB	1:A:385:ARG:HH22	1.83	0.43
1:C:394:LEU:O	1:C:398:ARG:HA	2.18	0.43
1:C:635:PHE:CE2	1:C:673:ALA:HB1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:GLU:OE1	1:B:557:SER:OG	2.35	0.43
1:D:541:PRO:HB2	1:D:542:GLN:H	1.64	0.43
1:A:434:TYR:CE2	1:A:437:SER:HB2	2.54	0.42
1:C:326:ASP:HB2	1:C:474:THR:HB	2.00	0.42
1:B:594:LYS:HA	1:C:579:GLY:H	1.84	0.42
1:D:173:VAL:HB	1:D:367:PRO:HG3	2.01	0.42
1:A:65:GLU:HB2	1:A:87:LYS:HD2	2.01	0.42
1:C:112:PHE:HD1	1:C:347:MET:HB2	1.83	0.42
1:A:218:SER:HB2	1:A:516:ASN:HB3	2.01	0.42
1:A:479:TYR:C	1:A:482:PRO:HD2	2.45	0.42
1:B:173:VAL:HB	1:B:385:ARG:HH22	1.84	0.42
1:B:255:THR:OG1	1:B:257:ASP:OD1	2.33	0.42
1:B:326:ASP:HB2	1:B:474:THR:HB	2.01	0.42
1:D:101:VAL:HG11	1:D:192:ILE:HD12	2.00	0.42
1:B:479:TYR:C	1:B:482:PRO:HD2	2.45	0.42
1:D:707:PHE:C	1:D:709:GLU:H	2.28	0.42
1:D:225:HIS:CE1	1:D:481:GLN:HB3	2.55	0.42
1:C:115:TYR:HD2	1:C:118:TRP:HZ2	1.67	0.42
1:D:162:ARG:NH2	1:D:369:HIS:CE1	2.87	0.42
1:B:225:HIS:CE1	1:B:481:GLN:HB3	2.55	0.41
1:D:326:ASP:HB2	1:D:474:THR:HB	2.02	0.41
1:C:201:ASN:HB3	1:D:297:TRP:CE3	2.56	0.41
1:D:136:VAL:HG12	1:D:163:PHE:HA	2.02	0.41
1:A:326:ASP:HB2	1:A:474:THR:HB	2.01	0.41
1:A:566:ILE:HD12	1:A:597:LEU:HD11	2.01	0.41
1:C:646:PRO:N	1:C:647:ALA:HA	2.35	0.41
1:D:479:TYR:C	1:D:482:PRO:HD2	2.45	0.41
1:C:185:ALA:HB3	1:C:384:GLY:HA3	2.02	0.41
1:C:252:ARG:NH1	1:C:461:ARG:HD3	2.35	0.41
1:D:127:LEU:HD11	1:D:132:LYS:HZ3	1.85	0.41
1:D:163:PHE:HB2	1:D:170:PHE:O	2.20	0.41
1:C:260:SER:HB3	1:C:458:THR:CG2	2.51	0.41
1:D:234:ASN:HD21	1:D:558:ILE:HD11	1.86	0.41
1:D:389:TYR:HA	1:D:392:THR:HG22	2.01	0.41
1:D:499:ASN:HA	1:D:502:ARG:HD2	2.03	0.41
1:A:294:GLN:OE1	1:B:203:VAL:HG11	2.21	0.41
1:B:218:SER:HB2	1:B:516:ASN:HB3	2.02	0.41
1:C:398:ARG:NH1	1:D:398:ARG:HG2	2.36	0.41
1:D:100:VAL:CG1	2:D:4000:HEM:HMA3	2.51	0.41
1:A:667:VAL:HG22	1:A:694:VAL:HG21	2.02	0.41
1:C:139:ARG:HD3	2:C:4000:HEM:O2A	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLU:HA	1:D:396:ARG:HH21	1.85	0.41
1:C:363:ILE:HD12	1:C:407:ILE:HG13	2.03	0.41
1:B:701:GLY:HA2	1:B:707:PHE:HZ	1.86	0.41
1:A:225:HIS:CE1	1:A:481:GLN:HB3	2.57	0.40
1:D:657:GLY:HA2	1:D:662:LYS:HD2	2.03	0.40
1:A:112:PHE:HD1	1:A:347:MET:HB2	1.86	0.40
1:A:185:ALA:HB3	1:A:384:GLY:HA3	2.03	0.40
2:C:4000:HEM:HMB1	2:C:4000:HEM:HBB2	2.02	0.40
1:D:140:PHE:HE1	1:D:159:PHE:CZ	2.39	0.40
1:D:653:ILE:O	1:D:656:ASP:O	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2016:HOH:O	3:D:2016:HOH:O[8_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	679/746 (91%)	640 (94%)	38 (6%)	1 (0%)	48	72
1	B	677/746 (91%)	628 (93%)	46 (7%)	3 (0%)	30	53
1	C	679/746 (91%)	619 (91%)	49 (7%)	11 (2%)	7	21
1	D	678/746 (91%)	585 (86%)	70 (10%)	23 (3%)	3	7
All	All	2713/2984 (91%)	2472 (91%)	203 (8%)	38 (1%)	9	24

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	THR
1	C	568	THR
1	D	427	ILE
1	D	563	LEU
1	D	564	PRO
1	D	705	PHE
1	B	632	GLU
1	C	152	THR
1	C	398	ARG
1	C	678	GLY
1	D	94	GLU
1	D	259	LYS
1	D	411	VAL
1	D	415	HIS
1	D	428	HIS
1	D	541	PRO
1	B	570	ARG
1	C	40	ARG
1	C	169	ASN
1	D	143	VAL
1	D	410	PRO
1	D	469	ARG
1	D	699	GLU
1	D	704	VAL
1	A	670	ALA
1	B	441	LYS
1	D	127	LEU
1	D	607	ALA
1	D	610	VAL
1	C	38	ASP
1	C	129	ALA
1	C	542	GLN
1	D	167	GLU
1	C	715	GLY
1	D	419	ARG
1	D	420	ASP
1	D	431	ILE
1	D	460	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar

resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/609 (92%)	515 (92%)	44 (8%)	11	29
1	B	557/609 (92%)	500 (90%)	57 (10%)	7	20
1	C	559/609 (92%)	490 (88%)	69 (12%)	4	14
1	D	558/609 (92%)	465 (83%)	93 (17%)	2	6
All	All	2233/2436 (92%)	1970 (88%)	263 (12%)	5	15

All (263) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LYS
1	A	64	GLU
1	A	65	GLU
1	A	96	ILE
1	A	146	SER
1	A	147	ARG
1	A	182	ILE
1	A	202	GLU
1	A	227	LEU
1	A	236	ILE
1	A	244	ASP
1	A	263	VAL
1	A	296	LEU
1	A	301	GLU
1	A	315	ILE
1	A	332	LYS
1	A	337	GLU
1	A	363	ILE
1	A	370	ILE
1	A	420	ASP
1	A	433	HIS
1	A	441	LYS
1	A	471	LEU
1	A	474	THR
1	A	483	ARG
1	A	511	GLU
1	A	538	LEU

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Mol	Chain	Res	Type
1	A	539	GLU
1	A	558	ILE
1	A	582	LEU
1	A	588	LEU
1	A	592	LEU
1	A	594	LYS
1	A	611	ASP
1	A	659	ARG
1	A	671	LYS
1	A	680	GLU
1	A	681	GLU
1	A	682	LYS
1	A	691	GLN
1	A	700	GLU
1	A	706	LYS
1	A	709	GLU
1	B	41	GLN
1	B	42	ARG
1	B	43	LEU
1	B	45	GLU
1	B	65	GLU
1	B	96	ILE
1	B	130	LYS
1	B	146	SER
1	B	166	ASP
1	B	182	ILE
1	B	202	GLU
1	B	227	LEU
1	B	236	ILE
1	B	244	ASP
1	B	263	VAL
1	B	296	LEU
1	B	301	GLU
1	B	315	ILE
1	B	332	LYS
1	B	337	GLU
1	B	363	ILE
1	B	370	ILE
1	B	411	VAL
1	B	418	HIS
1	B	419	ARG
1	B	431	ILE

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Mol	Chain	Res	Type
1	B	433	HIS
1	B	440	ASN
1	B	441	LYS
1	B	471	LEU
1	B	474	THR
1	B	539	GLU
1	B	542	GLN
1	B	563	LEU
1	B	566	ILE
1	B	569	LEU
1	B	570	ARG
1	B	578	LYS
1	B	582	LEU
1	B	584	LYS
1	B	588	LEU
1	B	591	GLN
1	B	592	LEU
1	B	611	ASP
1	B	632	GLU
1	B	633	ARG
1	B	638	LYS
1	B	659	ARG
1	B	671	LYS
1	B	672	LYS
1	B	677	ILE
1	B	680	GLU
1	B	687	TYR
1	B	696	LYS
1	B	699	GLU
1	B	706	LYS
1	B	709	GLU
1	C	36	GLU
1	C	48	VAL
1	C	51	ASN
1	C	63	ILE
1	C	78	LEU
1	C	79	LEU
1	C	80	GLU
1	C	85	ARG
1	C	94	GLU
1	C	96	ILE
1	C	111	ILE

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Mol	Chain	Res	Type
1	C	139	ARG
1	C	146	SER
1	C	151	ASP
1	C	154	ARG
1	C	155	ASP
1	C	156	VAL
1	C	167	GLU
1	C	182	ILE
1	C	202	GLU
1	C	227	LEU
1	C	236	ILE
1	C	239	SER
1	C	263	VAL
1	C	296	LEU
1	C	301	GLU
1	C	315	ILE
1	C	336	GLU
1	C	337	GLU
1	C	363	ILE
1	C	370	ILE
1	C	392	THR
1	C	393	GLN
1	C	394	LEU
1	C	395	ASN
1	C	409	ARG
1	C	419	ARG
1	C	422	GLN
1	C	424	GLN
1	C	441	LYS
1	C	450	THR
1	C	471	LEU
1	C	474	THR
1	C	511	GLU
1	C	538	LEU
1	C	552	VAL
1	C	558	ILE
1	C	566	ILE
1	C	570	ARG
1	C	582	LEU
1	C	588	LEU
1	C	590	GLU
1	C	592	LEU

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Mol	Chain	Res	Type
1	C	597	LEU
1	C	599	VAL
1	C	606	LEU
1	C	611	ASP
1	C	625	VAL
1	C	659	ARG
1	C	662	LYS
1	C	674	LEU
1	C	675	GLN
1	C	677	ILE
1	C	681	GLU
1	C	696	LYS
1	C	698	VAL
1	C	702	LEU
1	C	703	LYS
1	C	706	LYS
1	D	40	ARG
1	D	43	LEU
1	D	44	LYS
1	D	45	GLU
1	D	53	GLN
1	D	65	GLU
1	D	86	GLN
1	D	94	GLU
1	D	96	ILE
1	D	101	VAL
1	D	120	ASN
1	D	126	PHE
1	D	127	LEU
1	D	131	ASP
1	D	146	SER
1	D	166	ASP
1	D	167	GLU
1	D	183	GLN
1	D	184	ASP
1	D	190	ASP
1	D	193	HIS
1	D	202	GLU
1	D	227	LEU
1	D	236	ILE
1	D	238	ARG
1	D	244	ASP

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Mol	Chain	Res	Type
1	D	248	ILE
1	D	259	LYS
1	D	260	SER
1	D	263	VAL
1	D	279	GLU
1	D	296	LEU
1	D	301	GLU
1	D	304	ASN
1	D	315	ILE
1	D	316	ASP
1	D	321	GLN
1	D	332	LYS
1	D	337	GLU
1	D	343	VAL
1	D	370	ILE
1	D	381	LEU
1	D	386	LEU
1	D	393	GLN
1	D	394	LEU
1	D	420	ASP
1	D	427	ILE
1	D	429	LYS
1	D	431	ILE
1	D	432	HIS
1	D	433	HIS
1	D	439	LEU
1	D	440	ASN
1	D	453	ARG
1	D	461	ARG
1	D	467	LEU
1	D	469	ARG
1	D	470	GLU
1	D	474	THR
1	D	478	HIS
1	D	502	ARG
1	D	528	VAL
1	D	538	LEU
1	D	539	GLU
1	D	560	ASN
1	D	561	GLU
1	D	563	LEU
1	D	565	THR

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Mol	Chain	Res	Type
1	D	566	ILE
1	D	569	LEU
1	D	570	ARG
1	D	586	LYS
1	D	588	LEU
1	D	591	GLN
1	D	592	LEU
1	D	593	GLU
1	D	595	ASP
1	D	597	LEU
1	D	598	LYS
1	D	606	LEU
1	D	632	GLU
1	D	638	LYS
1	D	649	ARG
1	D	651	SER
1	D	652	GLN
1	D	659	ARG
1	D	672	LYS
1	D	691	GLN
1	D	695	ILE
1	D	698	VAL
1	D	700	GLU
1	D	702	LEU
1	D	706	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	352	ASN
1	A	362	GLN
1	A	401	ASN
1	A	417	ASN
1	A	418	HIS
1	A	487	ASN
1	A	520	GLN
1	A	591	GLN
1	A	612	GLN
1	B	169	ASN
1	B	234	ASN
1	B	282	GLN

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Mol	Chain	Res	Type
1	B	362	GLN
1	B	395	ASN
1	B	415	HIS
1	B	440	ASN
1	B	449	GLN
1	B	487	ASN
1	B	520	GLN
1	B	612	GLN
1	B	675	GLN
1	C	86	GLN
1	C	90	HIS
1	C	176	ASN
1	C	294	GLN
1	C	393	GLN
1	C	395	ASN
1	C	401	ASN
1	C	424	GLN
1	C	478	HIS
1	C	487	ASN
1	C	520	GLN
1	C	522	ASN
1	C	526	ASN
1	C	652	GLN
1	C	691	GLN
1	D	41	GLN
1	D	86	GLN
1	D	90	HIS
1	D	183	GLN
1	D	234	ASN
1	D	304	ASN
1	D	350	ASN
1	D	362	GLN
1	D	416	ASN
1	D	417	ASN
1	D	418	HIS
1	D	468	ASN
1	D	487	ASN
1	D	520	GLN
1	D	612	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	B	4000	1	50,50,50	1.45	9 (18%)	67,82,82	1.46	10 (14%)
2	HEM	C	4000	1	50,50,50	1.43	7 (14%)	67,82,82	1.44	12 (17%)
2	HEM	D	4000	-	50,50,50	1.55	11 (22%)	67,82,82	1.58	15 (22%)
2	HEM	A	4000	1	50,50,50	1.45	8 (16%)	67,82,82	1.46	12 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	4000	1	-	2/14/54/54	-
2	HEM	C	4000	1	-	2/14/54/54	-
2	HEM	D	4000	-	-	5/14/54/54	-
2	HEM	A	4000	1	-	2/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4000	HEM	O1D-CGD	4.36	1.36	1.22
2	A	4000	HEM	C4D-ND	-4.31	1.32	1.40
2	C	4000	HEM	C4D-ND	-4.06	1.33	1.40
2	B	4000	HEM	C4D-ND	-3.88	1.33	1.40
2	C	4000	HEM	C1B-NB	-3.68	1.33	1.40
2	B	4000	HEM	C1B-NB	-3.44	1.34	1.40
2	A	4000	HEM	C1B-NB	-3.31	1.34	1.40
2	A	4000	HEM	C1C-C2C	-3.23	1.39	1.45
2	D	4000	HEM	C4D-C3D	3.22	1.50	1.45
2	D	4000	HEM	C1B-NB	-3.16	1.34	1.40
2	B	4000	HEM	C3D-C2D	-2.99	1.30	1.36
2	A	4000	HEM	C3D-C2D	-2.96	1.30	1.36
2	B	4000	HEM	C4B-NB	-2.91	1.33	1.38
2	D	4000	HEM	O2D-CGD	-2.82	1.21	1.30
2	D	4000	HEM	C3B-C4B	2.71	1.50	1.44
2	D	4000	HEM	C1D-C2D	2.67	1.49	1.44
2	B	4000	HEM	C4D-C3D	2.51	1.49	1.45
2	D	4000	HEM	C3B-C2B	-2.50	1.32	1.37
2	A	4000	HEM	C3B-C4B	2.49	1.49	1.44
2	C	4000	HEM	C4B-NB	-2.49	1.34	1.38
2	C	4000	HEM	C1D-ND	-2.49	1.34	1.38
2	A	4000	HEM	C4B-NB	-2.48	1.34	1.38
2	B	4000	HEM	C1D-C2D	2.40	1.49	1.44
2	B	4000	HEM	C1D-ND	-2.40	1.34	1.38
2	A	4000	HEM	C1D-ND	-2.33	1.34	1.38
2	C	4000	HEM	C3D-C2D	-2.33	1.31	1.36
2	D	4000	HEM	C3C-C4C	-2.30	1.42	1.46
2	D	4000	HEM	C4B-NB	-2.25	1.34	1.38
2	D	4000	HEM	CHA-C1A	-2.24	1.34	1.39
2	D	4000	HEM	C4D-ND	-2.23	1.36	1.40
2	B	4000	HEM	C1C-C2C	-2.18	1.41	1.45
2	B	4000	HEM	CHB-C4A	-2.17	1.34	1.39
2	C	4000	HEM	C3B-C4B	2.15	1.49	1.44
2	C	4000	HEM	C1C-C2C	-2.13	1.41	1.45
2	A	4000	HEM	CAC-C3C	2.08	1.52	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4000	HEM	CAD-CBD-CGD	-4.63	101.39	113.67
2	A	4000	HEM	C4B-C3B-C2B	-4.11	103.50	107.28
2	D	4000	HEM	CMB-C2B-C1B	3.91	131.14	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4000	HEM	C4B-C3B-C2B	-3.79	103.80	107.28
2	B	4000	HEM	C3B-C4B-NB	3.42	111.92	109.47
2	C	4000	HEM	C4B-C3B-C2B	-3.32	104.22	107.28
2	D	4000	HEM	C2D-C1D-ND	3.29	113.71	109.90
2	B	4000	HEM	CHD-C1D-C2D	-3.07	120.18	125.03
2	C	4000	HEM	C4C-C3C-C2C	-2.92	104.28	106.81
2	D	4000	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
2	C	4000	HEM	CHD-C1D-C2D	-2.89	120.46	125.03
2	A	4000	HEM	C3B-C4B-NB	2.85	111.52	109.47
2	D	4000	HEM	C2B-C1B-NB	2.79	113.05	109.84
2	B	4000	HEM	CBD-CAD-C3D	-2.72	105.02	112.53
2	A	4000	HEM	CHC-C4B-NB	2.63	127.25	124.42
2	C	4000	HEM	C1D-C2D-C3D	-2.61	104.23	106.98
2	C	4000	HEM	C2B-C1B-NB	2.61	112.84	109.84
2	C	4000	HEM	CBD-CAD-C3D	-2.59	105.37	112.53
2	C	4000	HEM	CHD-C1D-ND	2.56	127.18	124.42
2	B	4000	HEM	CHD-C1D-ND	2.56	127.18	124.42
2	A	4000	HEM	C2B-C1B-NB	2.55	112.77	109.84
2	D	4000	HEM	CMA-C3A-C2A	2.55	131.02	125.62
2	A	4000	HEM	CMA-C3A-C2A	2.53	131.00	125.62
2	A	4000	HEM	CHD-C1D-C2D	-2.49	121.09	125.03
2	C	4000	HEM	CMA-C3A-C2A	2.48	130.89	125.62
2	B	4000	HEM	O2D-CGD-CBD	2.47	121.81	114.00
2	A	4000	HEM	CBD-CAD-C3D	-2.47	105.70	112.53
2	B	4000	HEM	CMA-C3A-C2A	2.41	130.74	125.62
2	D	4000	HEM	C3B-C4B-NB	2.40	111.19	109.47
2	B	4000	HEM	C4C-CHD-C1D	-2.38	120.97	126.02
2	B	4000	HEM	C2D-C1D-ND	2.37	112.64	109.90
2	B	4000	HEM	C1D-C2D-C3D	-2.37	104.49	106.98
2	D	4000	HEM	CMB-C2B-C3B	-2.31	122.83	128.43
2	D	4000	HEM	C3D-C4D-ND	2.30	112.70	110.17
2	A	4000	HEM	C2D-C1D-ND	2.25	112.50	109.90
2	D	4000	HEM	C2A-C1A-NA	2.25	112.65	110.15
2	D	4000	HEM	C4C-CHD-C1D	-2.23	121.28	126.02
2	C	4000	HEM	C3B-C4B-NB	2.21	111.06	109.47
2	C	4000	HEM	CHC-C4B-NB	2.21	126.80	124.42
2	A	4000	HEM	C4C-C3C-C2C	-2.20	104.91	106.81
2	A	4000	HEM	C1D-C2D-C3D	-2.18	104.69	106.98
2	C	4000	HEM	O2D-CGD-CBD	2.17	120.87	114.00
2	D	4000	HEM	C4D-ND-C1D	-2.17	102.63	105.21
2	A	4000	HEM	O2D-CGD-CBD	2.17	120.87	114.00
2	D	4000	HEM	C1D-C2D-C3D	-2.13	104.74	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	HEM	CHC-C1C-C2C	-2.12	121.08	125.49
2	C	4000	HEM	C2D-C1D-ND	2.11	112.34	109.90
2	D	4000	HEM	CHC-C4B-NB	2.09	126.68	124.42
2	D	4000	HEM	CHA-C4D-C3D	-2.02	121.51	125.23

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	4000	HEM	C2B-C3B-CAB-CBB
2	D	4000	HEM	C4B-C3B-CAB-CBB
2	A	4000	HEM	CAA-CBA-CGA-O2A
2	B	4000	HEM	CAA-CBA-CGA-O2A
2	D	4000	HEM	CAD-CBD-CGD-O1D
2	C	4000	HEM	CAA-CBA-CGA-O2A
2	B	4000	HEM	CAA-CBA-CGA-O1A
2	C	4000	HEM	CAA-CBA-CGA-O1A
2	D	4000	HEM	CAD-CBD-CGD-O2D
2	A	4000	HEM	CAA-CBA-CGA-O1A
2	D	4000	HEM	C4C-C3C-CAC-CBC

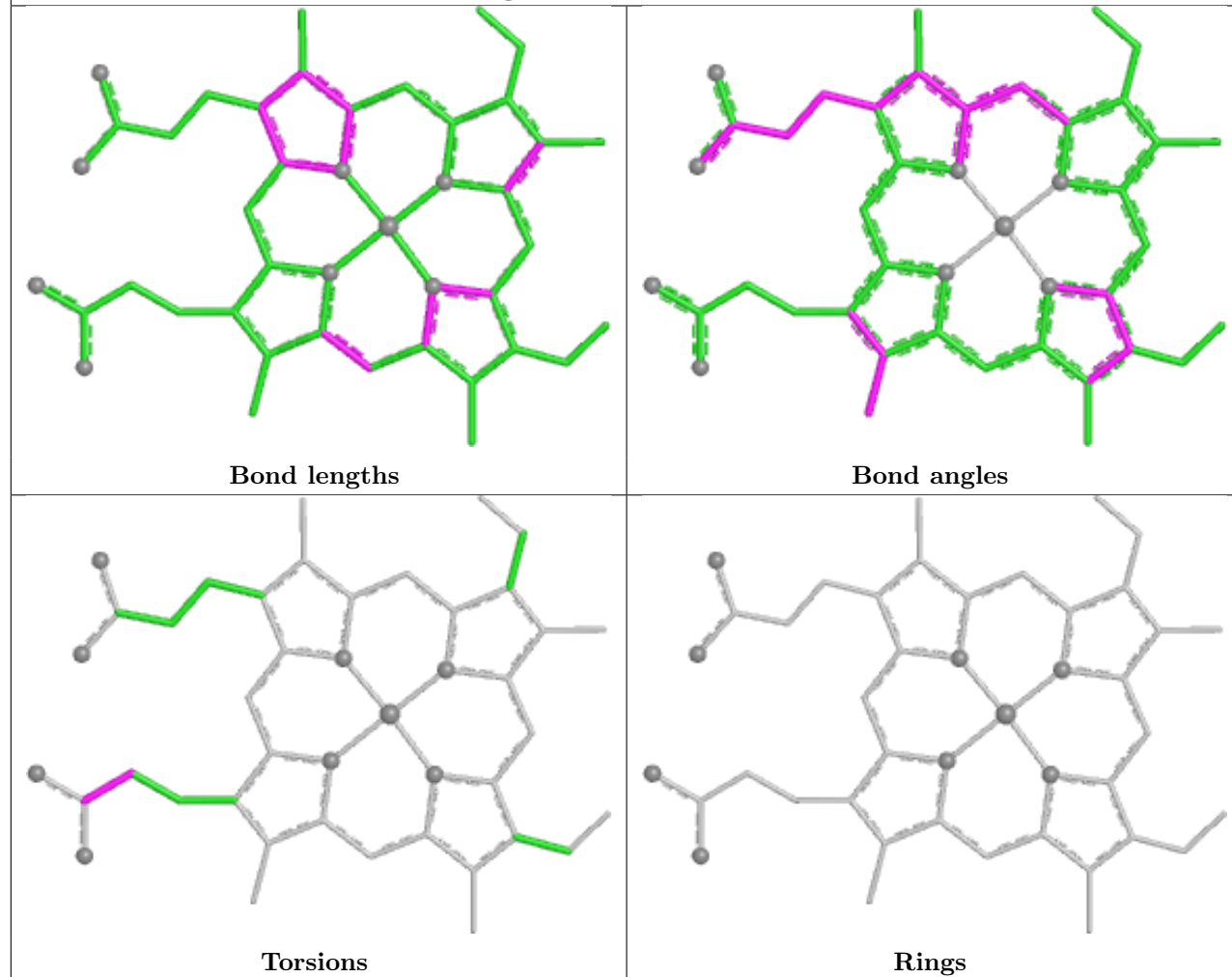
There are no ring outliers.

4 monomers are involved in 7 short contacts:

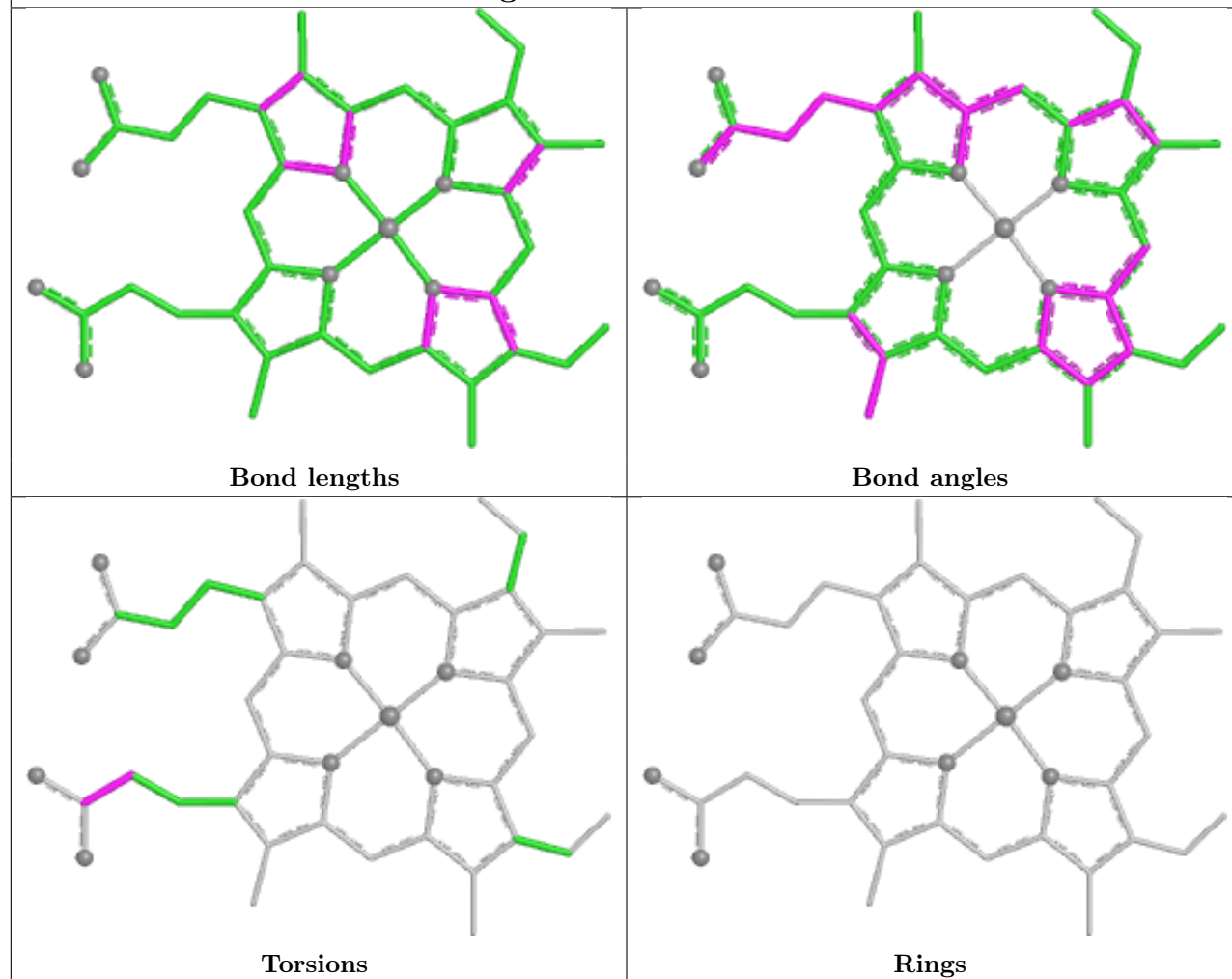
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	4000	HEM	1	0
2	C	4000	HEM	3	0
2	D	4000	HEM	2	0
2	A	4000	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

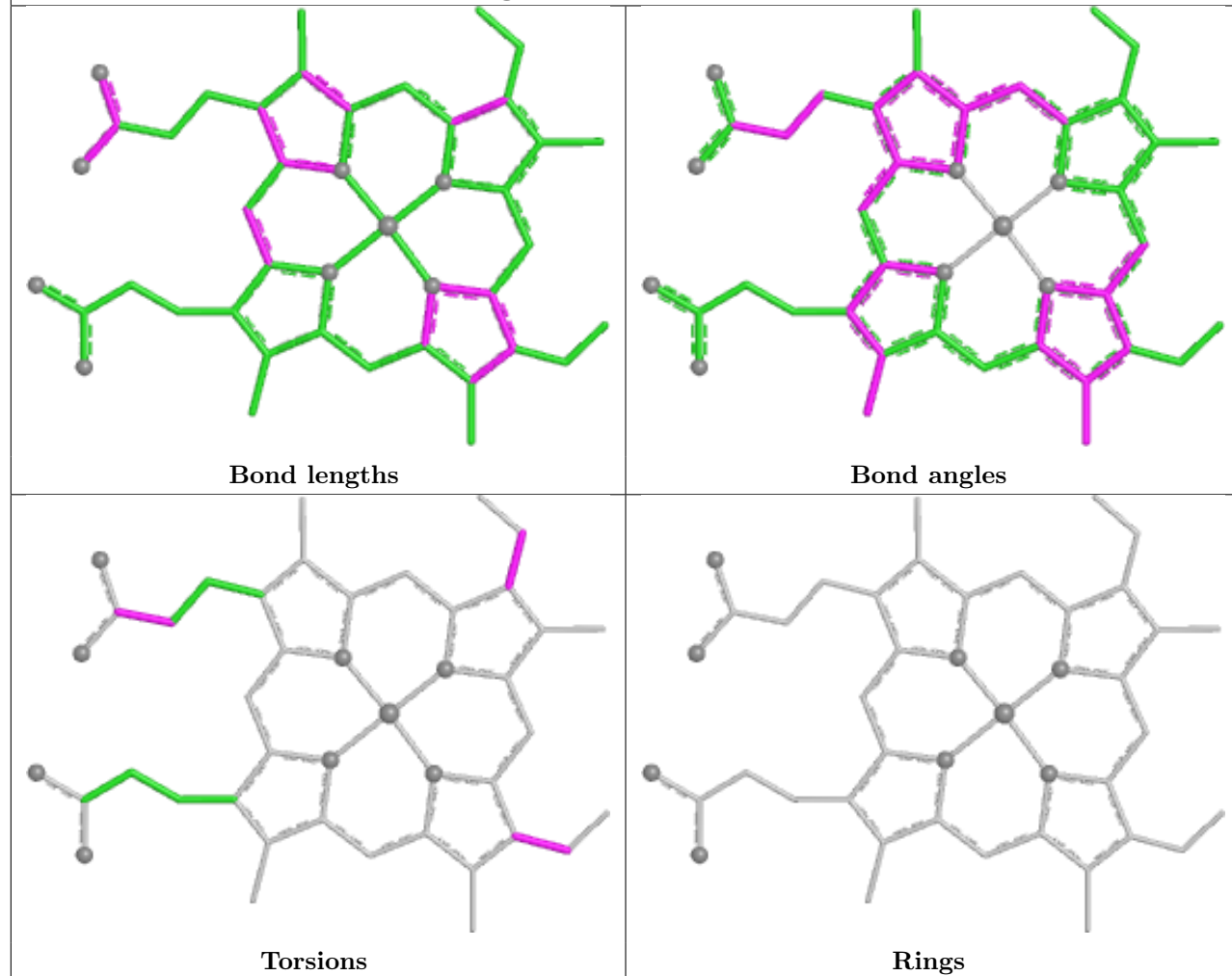
Ligand HEM B 4000

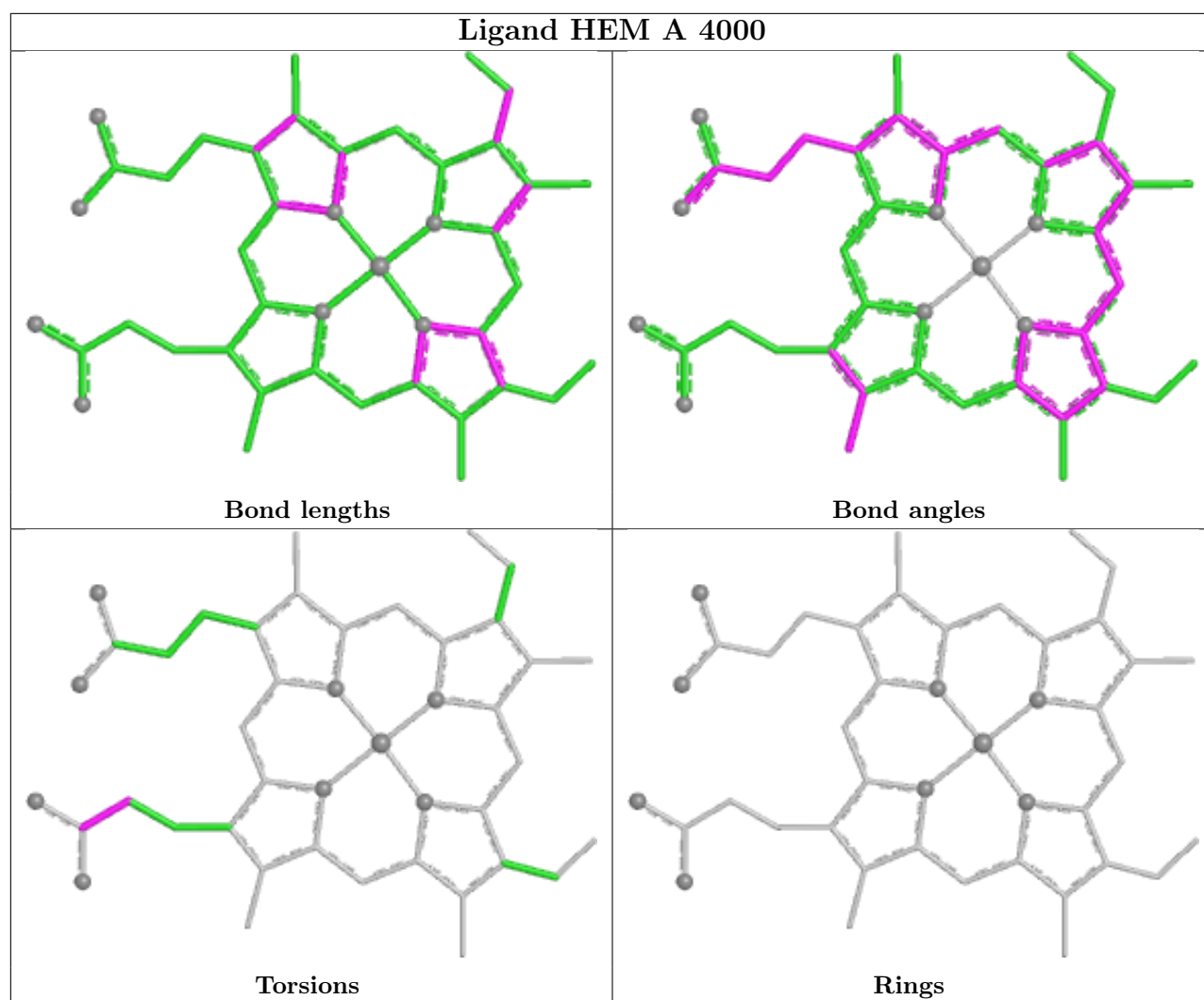


Ligand HEM C 4000



Ligand HEM D 4000





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	681/746 (91%)	0.35	22 (3%)	50	43	15, 51, 103, 141	0
1	B	679/746 (91%)	0.74	81 (11%)	9	8	19, 63, 154, 227	0
1	C	681/746 (91%)	1.81	264 (38%)	1	0	32, 79, 138, 169	0
1	D	680/746 (91%)	2.49	443 (65%)	0	0	32, 94, 149, 188	0
All	All	2721/2984 (91%)	1.35	810 (29%)	1	1	15, 75, 140, 227	0

All (810) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	624	ALA	8.0
1	D	664	VAL	7.1
1	C	360	THR	7.1
1	D	434	TYR	6.6
1	B	686	VAL	6.5
1	C	572	GLY	6.4
1	C	88	LEU	6.4
1	D	418	HIS	6.3
1	C	79	LEU	6.3
1	C	626	VAL	6.2
1	C	623	ASP	6.2
1	D	388	SER	6.1
1	C	708	LEU	6.1
1	D	314	LEU	6.0
1	B	687	TYR	5.7
1	D	444	PRO	5.6
1	D	687	TYR	5.6
1	C	82	PHE	5.6
1	D	283	VAL	5.6
1	D	223	ALA	5.6
1	C	573	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	370	ILE	5.5
1	D	190	ASP	5.5
1	C	78	LEU	5.4
1	D	455	PHE	5.4
1	C	63	ILE	5.4
1	D	193	HIS	5.4
1	D	433	HIS	5.4
1	B	568	THR	5.3
1	D	431	ILE	5.2
1	D	400	PRO	5.2
1	D	436	PRO	5.2
1	C	605	TYR	5.2
1	C	158	GLY	5.2
1	C	579	GLY	5.2
1	D	311	ALA	5.2
1	C	625	VAL	5.1
1	D	439	LEU	5.1
1	D	556	VAL	5.1
1	C	428	HIS	5.1
1	D	228	PHE	5.1
1	D	376	PHE	5.1
1	C	161	THR	5.0
1	D	143	VAL	5.0
1	B	685	GLY	4.9
1	D	432	HIS	4.9
1	D	501	ILE	4.9
1	D	482	PRO	4.9
1	D	698	VAL	4.9
1	D	121	ILE	4.9
1	D	225	HIS	4.9
1	D	110	GLY	4.8
1	D	422	GLN	4.8
1	D	224	LEU	4.8
1	D	467	LEU	4.8
1	C	571	VAL	4.8
1	C	677	ILE	4.8
1	C	69	LEU	4.7
1	D	371	VAL	4.7
1	C	619	ALA	4.7
1	D	150	ALA	4.7
1	D	238	ARG	4.7
1	D	304	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	90	HIS	4.7
1	C	645	PHE	4.7
1	D	333	PHE	4.7
1	B	545	PRO	4.6
1	C	427	ILE	4.6
1	D	374	VAL	4.6
1	D	170	PHE	4.6
1	D	574	LEU	4.5
1	D	353	PRO	4.5
1	D	368	GLY	4.5
1	D	416	ASN	4.5
1	C	653	ILE	4.5
1	D	435	SER	4.5
1	B	695	ILE	4.5
1	D	545	PRO	4.5
1	D	383	GLN	4.5
1	C	644	LEU	4.5
1	C	84	PHE	4.5
1	C	80	GLU	4.4
1	C	651	SER	4.4
1	D	406	PRO	4.4
1	D	447	ALA	4.4
1	B	679	VAL	4.4
1	C	627	VAL	4.4
1	D	625	VAL	4.4
1	D	597	LEU	4.4
1	B	588	LEU	4.4
1	C	96	ILE	4.4
1	D	589	LYS	4.3
1	D	485	PHE	4.3
1	C	83	ILE	4.3
1	B	698	VAL	4.3
1	D	624	ALA	4.3
1	D	352	ASN	4.3
1	D	367	PRO	4.3
1	D	233	GLY	4.3
1	D	249	HIS	4.3
1	D	600	THR	4.3
1	C	66	GLN	4.3
1	D	701	GLY	4.3
1	D	525	SER	4.2
1	D	242	HIS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	598	LYS	4.2
1	C	81	ASP	4.2
1	D	426	TRP	4.2
1	C	676	SER	4.2
1	D	665	ALA	4.2
1	D	214	TRP	4.2
1	D	453	ARG	4.2
1	D	349	LEU	4.2
1	D	454	GLY	4.2
1	D	377	THR	4.1
1	D	402	PHE	4.2
1	D	559	PHE	4.1
1	D	552	VAL	4.1
1	C	655	THR	4.1
1	D	674	LEU	4.1
1	B	684	ALA	4.1
1	D	438	TYR	4.1
1	C	60	GLY	4.1
1	D	315	ILE	4.1
1	C	59	PHE	4.1
1	D	457	THR	4.1
1	B	665	ALA	4.1
1	D	206	ALA	4.1
1	C	239	SER	4.1
1	D	108	ALA	4.0
1	C	417	ASN	4.0
1	D	437	SER	4.0
1	D	405	LEU	4.0
1	C	637	GLY	4.0
1	D	452	GLY	4.0
1	B	694	VAL	4.0
1	D	215	ASP	4.0
1	C	43	LEU	4.0
1	C	687	TYR	4.0
1	C	284	LEU	4.0
1	B	691	GLN	4.0
1	D	123	ALA	3.9
1	D	566	ILE	3.9
1	C	154	ARG	3.9
1	D	588	LEU	3.9
1	D	182	ILE	3.9
1	C	71	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	281	ALA	3.9
1	D	628	ALA	3.9
1	C	610	VAL	3.9
1	D	411	VAL	3.9
1	B	689	GLY	3.8
1	D	227	LEU	3.8
1	D	365	PHE	3.8
1	D	192	ILE	3.8
1	C	425	ALA	3.8
1	D	153	ALA	3.8
1	B	592	LEU	3.8
1	D	569	LEU	3.8
1	D	335	PRO	3.8
1	C	160	ALA	3.8
1	C	539	GLU	3.8
1	D	407	ILE	3.8
1	B	567	ALA	3.8
1	C	39	ALA	3.8
1	C	77	THR	3.8
1	C	74	ARG	3.7
1	D	312	VAL	3.7
1	D	414	VAL	3.7
1	C	426	TRP	3.7
1	D	690	ALA	3.7
1	A	665	ALA	3.7
1	D	358	ALA	3.7
1	C	648	GLY	3.7
1	D	399	GLY	3.7
1	C	642	SER	3.7
1	D	292	HIS	3.7
1	D	325	PHE	3.7
1	D	622	PHE	3.7
1	D	564	PRO	3.7
1	D	592	LEU	3.7
1	C	67	PHE	3.7
1	D	176	ASN	3.7
1	C	150	ALA	3.6
1	D	419	ARG	3.6
1	C	588	LEU	3.6
1	D	217	PHE	3.6
1	C	48	VAL	3.6
1	D	240	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	230	ALA	3.6
1	B	586	LYS	3.6
1	D	194	SER	3.6
1	C	91	PHE	3.6
1	D	695	ILE	3.6
1	D	251	PHE	3.6
1	B	539	GLU	3.6
1	C	58	ASP	3.6
1	D	379	ASP	3.6
1	C	390	LEU	3.6
1	D	347	MET	3.6
1	D	563	LEU	3.6
1	B	540	ALA	3.5
1	B	688	ALA	3.5
1	C	85	ARG	3.5
1	D	236	ILE	3.5
1	D	427	ILE	3.5
1	B	573	VAL	3.5
1	C	157	HIS	3.5
1	D	41	GLN	3.5
1	C	237	PRO	3.5
1	D	417	ASN	3.5
1	D	456	PHE	3.5
1	D	263	VAL	3.5
1	B	683	GLU	3.5
1	C	202	GLU	3.5
1	C	674	LEU	3.5
1	C	50	ASP	3.5
1	D	246	PHE	3.5
1	C	698	VAL	3.5
1	D	132	LYS	3.5
1	C	68	SER	3.5
1	D	212	SER	3.5
1	D	459	PRO	3.5
1	C	617	ALA	3.5
1	C	621	ALA	3.5
1	D	602	ILE	3.4
1	C	283	VAL	3.4
1	D	575	SER	3.4
1	D	387	TYR	3.4
1	D	140	PHE	3.4
1	B	697	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	596	GLY	3.4
1	C	640	ALA	3.4
1	C	356	TYR	3.4
1	D	356	TYR	3.4
1	D	713	VAL	3.4
1	D	252	ARG	3.4
1	D	375	ASP	3.4
1	D	524	ILE	3.4
1	C	127	LEU	3.4
1	C	203	VAL	3.4
1	D	310	LEU	3.4
1	D	396	ARG	3.4
1	D	198	SER	3.4
1	D	297	TRP	3.4
1	D	389	TYR	3.4
1	D	296	LEU	3.3
1	C	659	ARG	3.3
1	C	89	GLN	3.3
1	C	652	GLN	3.3
1	D	142	THR	3.3
1	C	634	VAL	3.3
1	C	682	LYS	3.3
1	B	640	ALA	3.3
1	C	358	ALA	3.3
1	D	122	THR	3.3
1	D	568	THR	3.3
1	D	136	VAL	3.3
1	D	451	VAL	3.3
1	D	384	GLY	3.3
1	D	423	GLY	3.3
1	C	62	ASN	3.3
1	B	699	GLU	3.3
1	C	199	PRO	3.3
1	D	673	ALA	3.3
1	C	137	PHE	3.3
1	D	208	THR	3.3
1	D	497	VAL	3.3
1	C	49	ASP	3.3
1	D	317	GLU	3.3
1	D	644	LEU	3.3
1	D	492	VAL	3.3
1	D	474	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	693	GLU	3.2
1	D	126	PHE	3.2
1	D	137	PHE	3.2
1	D	282	GLN	3.2
1	C	73	GLY	3.2
1	C	345	GLY	3.2
1	D	623	ASP	3.2
1	D	127	LEU	3.2
1	A	698	VAL	3.2
1	B	634	VAL	3.2
1	C	419	ARG	3.2
1	D	103	ALA	3.2
1	D	684	ALA	3.2
1	C	86	GLN	3.2
1	C	672	LYS	3.2
1	D	313	GLN	3.2
1	C	65	GLU	3.2
1	D	114	SER	3.2
1	D	677	ILE	3.2
1	B	569	LEU	3.2
1	D	445	ALA	3.2
1	C	622	PHE	3.2
1	C	667	VAL	3.2
1	D	679	VAL	3.2
1	D	300	ILE	3.2
1	D	491	PRO	3.2
1	D	440	ASN	3.1
1	D	338	PHE	3.1
1	D	571	VAL	3.1
1	C	691	GLN	3.1
1	D	360	THR	3.1
1	C	111	ILE	3.1
1	C	574	LEU	3.1
1	C	496	PHE	3.1
1	D	188	PHE	3.1
1	D	100	VAL	3.1
1	D	639	GLY	3.1
1	D	697	GLY	3.1
1	D	450	THR	3.1
1	D	267	TRP	3.1
1	D	285	ALA	3.1
1	D	443	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	587	ALA	3.1
1	D	222	SER	3.1
1	C	40	ARG	3.1
1	D	207	ALA	3.1
1	D	265	TRP	3.1
1	D	308	TRP	3.1
1	C	694	VAL	3.1
1	D	291	PHE	3.1
1	D	517	VAL	3.1
1	A	630	GLY	3.1
1	C	64	GLU	3.1
1	C	238	ARG	3.1
1	C	671	LYS	3.1
1	D	390	LEU	3.1
1	C	647	ALA	3.0
1	C	366	GLN	3.0
1	D	558	ILE	3.0
1	B	696	LYS	3.0
1	D	577	THR	3.0
1	D	124	ALA	3.0
1	D	425	ALA	3.0
1	D	621	ALA	3.0
1	C	433	HIS	3.0
1	C	583	ASP	3.0
1	C	300	ILE	3.0
1	D	362	GLN	3.0
1	A	538	LEU	3.0
1	D	484	LEU	3.0
1	D	518	LEU	3.0
1	C	197	PRO	3.0
1	B	577	THR	3.0
1	C	277	VAL	3.0
1	C	365	PHE	3.0
1	C	664	VAL	3.0
1	C	265	TRP	3.0
1	C	308	TRP	3.0
1	C	558	ILE	3.0
1	C	570	ARG	3.0
1	D	40	ARG	3.0
1	D	446	GLN	3.0
1	D	702	LEU	3.0
1	C	56	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	93	HIS	3.0
1	C	363	ILE	3.0
1	C	107	GLY	3.0
1	C	116	GLY	3.0
1	D	260	SER	3.0
1	B	643	PRO	3.0
1	D	330	PRO	3.0
1	C	392	THR	3.0
1	D	397	HIS	3.0
1	C	689	GLY	2.9
1	D	334	LEU	2.9
1	D	220	GLN	2.9
1	D	171	ASP	2.9
1	C	635	PHE	2.9
1	D	216	PHE	2.9
1	D	458	THR	2.9
1	D	486	PHE	2.9
1	D	620	THR	2.9
1	C	675	GLN	2.9
1	D	508	VAL	2.9
1	D	540	ALA	2.9
1	C	695	ILE	2.9
1	D	96	ILE	2.9
1	C	52	GLY	2.9
1	D	117	ASP	2.9
1	D	155	ASP	2.9
1	D	401	ASN	2.9
1	D	146	SER	2.9
1	D	307	SER	2.9
1	D	640	ALA	2.9
1	D	651	SER	2.9
1	D	528	VAL	2.9
1	D	582	LEU	2.9
1	D	572	GLY	2.9
1	A	350	ASN	2.9
1	D	626	VAL	2.9
1	D	694	VAL	2.9
1	B	676	SER	2.9
1	D	109	HIS	2.9
1	D	502	ARG	2.9
1	C	654	LEU	2.9
1	D	380	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	614	TYR	2.8
1	B	690	ALA	2.8
1	D	532	VAL	2.8
1	D	448	ASN	2.8
1	D	567	ALA	2.8
1	C	618	ASP	2.8
1	D	527	ASP	2.8
1	D	141	SER	2.8
1	D	43	LEU	2.8
1	C	168	GLY	2.8
1	D	442	GLY	2.8
1	D	197	PRO	2.8
1	D	196	LYS	2.8
1	D	98	GLU	2.8
1	B	277	VAL	2.8
1	B	631	ALA	2.8
1	D	535	ALA	2.8
1	C	288	ASN	2.8
1	D	381	LEU	2.8
1	D	538	LEU	2.8
1	D	226	THR	2.8
1	D	135	PRO	2.8
1	D	189	PRO	2.8
1	D	393	GLN	2.8
1	D	520	GLN	2.8
1	B	593	GLU	2.8
1	B	605	TYR	2.8
1	C	679	VAL	2.8
1	A	588	LEU	2.8
1	A	702	LEU	2.8
1	B	677	ILE	2.8
1	D	565	THR	2.8
1	C	609	GLY	2.8
1	C	643	PRO	2.8
1	D	46	VAL	2.8
1	D	164	TYR	2.8
1	B	582	LEU	2.8
1	C	702	LEU	2.8
1	C	391	ASP	2.8
1	D	244	ASP	2.8
1	D	45	GLU	2.7
1	D	280	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	586	LYS	2.7
1	C	458	THR	2.7
1	D	340	PRO	2.7
1	D	481	GLN	2.7
1	D	712	ALA	2.7
1	D	548	TYR	2.7
1	C	142	THR	2.7
1	D	134	THR	2.7
1	D	152	THR	2.7
1	C	603	ALA	2.7
1	D	328	LEU	2.7
1	D	705	PHE	2.7
1	C	196	LYS	2.7
1	C	57	THR	2.7
1	C	165	THR	2.7
1	C	304	ASN	2.7
1	C	460	GLY	2.7
1	D	187	ARG	2.7
1	D	131	ASP	2.7
1	C	404	GLN	2.7
1	C	412	SER	2.7
1	C	156	VAL	2.7
1	D	361	GLU	2.7
1	D	276	LEU	2.7
1	C	106	ALA	2.7
1	D	241	ARG	2.7
1	C	204	PRO	2.7
1	D	169	ASN	2.7
1	D	468	ASN	2.7
1	D	553	THR	2.7
1	C	92	ASP	2.7
1	C	279	GLU	2.7
1	D	634	VAL	2.7
1	C	114	SER	2.7
1	C	606	LEU	2.7
1	D	111	ILE	2.6
1	D	412	SER	2.7
1	C	126	PHE	2.6
1	D	261	LYS	2.6
1	D	264	LYS	2.6
1	C	540	ALA	2.6
1	D	463	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	545	PRO	2.6
1	D	61	GLY	2.6
1	C	276	LEU	2.6
1	D	256	GLU	2.6
1	C	690	ALA	2.6
1	D	631	ALA	2.6
1	D	266	HIS	2.6
1	B	596	GLY	2.6
1	C	650	PRO	2.6
1	B	682	LYS	2.6
1	C	348	THR	2.6
1	D	392	THR	2.6
1	B	626	VAL	2.6
1	A	677	ILE	2.6
1	C	359	GLU	2.6
1	C	556	VAL	2.6
1	D	37	VAL	2.6
1	D	53	GLN	2.6
1	D	101	VAL	2.6
1	D	138	VAL	2.6
1	D	627	VAL	2.6
1	C	155	ASP	2.6
1	D	184	ASP	2.6
1	D	420	ASP	2.6
1	D	544	ASP	2.6
1	C	207	ALA	2.6
1	D	320	ALA	2.6
1	C	292	HIS	2.6
1	D	543	PRO	2.6
1	C	696	LYS	2.6
1	B	565	THR	2.6
1	D	195	VAL	2.6
1	D	513	VAL	2.6
1	C	120	ASN	2.6
1	D	209	ALA	2.6
1	D	219	SER	2.6
1	B	543	PRO	2.6
1	C	264	LYS	2.6
1	D	413	GLY	2.6
1	A	691	GLN	2.6
1	C	205	GLN	2.6
1	D	47	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	337	GLU	2.6
1	B	275	ALA	2.6
1	C	275	ALA	2.6
1	D	120	ASN	2.6
1	D	617	ALA	2.6
1	D	618	ASP	2.6
1	D	478	HIS	2.5
1	C	76	SER	2.5
1	D	259	LYS	2.5
1	B	297	TRP	2.5
1	D	599	VAL	2.5
1	D	704	VAL	2.5
1	B	542	GLN	2.5
1	D	496	PHE	2.5
1	D	503	PHE	2.5
1	D	611	ASP	2.5
1	A	671	LYS	2.5
1	C	569	LEU	2.5
1	C	604	GLU	2.5
1	C	246	PHE	2.5
1	C	282	GLN	2.5
1	D	112	PHE	2.5
1	D	710	ARG	2.5
1	B	574	LEU	2.5
1	C	582	LEU	2.5
1	D	191	LEU	2.5
1	D	708	LEU	2.5
1	B	639	GLY	2.5
1	C	685	GLY	2.5
1	C	297	TRP	2.5
1	C	660	TRP	2.5
1	D	573	VAL	2.5
1	D	605	TYR	2.5
1	D	163	PHE	2.5
1	C	299	ALA	2.5
1	D	129	ALA	2.5
1	D	255	THR	2.5
1	D	331	THR	2.5
1	C	578	LYS	2.5
1	D	578	LYS	2.5
1	D	151	ASP	2.5
1	D	386	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	536	LEU	2.5
1	C	537	GLY	2.5
1	D	218	SER	2.5
1	C	37	VAL	2.5
1	D	359	GLU	2.5
1	D	154	ARG	2.5
1	D	271	GLN	2.5
1	D	570	ARG	2.5
1	C	70	LYS	2.5
1	D	332	LYS	2.5
1	D	177	ILE	2.4
1	D	248	ILE	2.4
1	D	145	GLY	2.4
1	B	475	PHE	2.4
1	B	39	ALA	2.4
1	C	662	LYS	2.4
1	C	51	ASN	2.4
1	B	597	LEU	2.4
1	B	702	LEU	2.4
1	D	262	LEU	2.4
1	C	646	PRO	2.4
1	C	663	PRO	2.4
1	B	633	ARG	2.4
1	D	645	PHE	2.4
1	D	707	PHE	2.4
1	B	666	ALA	2.4
1	B	675	GLN	2.4
1	C	153	ALA	2.4
1	D	106	ALA	2.4
1	C	600	THR	2.4
1	C	408	ASN	2.4
1	D	395	ASN	2.4
1	C	491	PRO	2.4
1	D	178	PRO	2.4
1	D	203	VAL	2.4
1	D	706	LYS	2.4
1	B	681	GLU	2.4
1	C	54	PHE	2.4
1	C	364	SER	2.4
1	C	681	GLU	2.4
1	D	301	GLU	2.4
1	D	709	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	616	ALA	2.4
1	C	271	GLN	2.4
1	D	490	THR	2.4
1	B	599	VAL	2.4
1	C	599	VAL	2.4
1	B	692	ASP	2.4
1	C	151	ASP	2.4
1	D	477	ASP	2.4
1	A	540	ALA	2.4
1	C	108	ALA	2.4
1	D	585	ALA	2.4
1	C	636	SER	2.4
1	D	269	THR	2.4
1	D	327	LEU	2.4
1	C	407	ILE	2.4
1	D	696	LYS	2.3
1	D	475	PHE	2.3
1	C	94	GLU	2.3
1	C	587	ALA	2.3
1	C	688	ALA	2.3
1	B	125	SER	2.3
1	D	118	TRP	2.3
1	D	441	LYS	2.3
1	C	147	ARG	2.3
1	D	48	VAL	2.3
1	D	156	VAL	2.3
1	D	254	VAL	2.3
1	D	372	ARG	2.3
1	D	398	ARG	2.3
1	D	299	ALA	2.3
1	C	267	TRP	2.3
1	C	113	THR	2.3
1	D	576	THR	2.3
1	D	653	ILE	2.3
1	D	204	PRO	2.3
1	D	350	ASN	2.3
1	B	45	GLU	2.3
1	C	673	ALA	2.3
1	C	699	GLU	2.3
1	D	144	ALA	2.3
1	D	183	GLN	2.3
1	B	566	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	562	SER	2.3
1	D	348	THR	2.3
1	C	241	ARG	2.3
1	D	115	TYR	2.3
1	C	601	VAL	2.3
1	D	289	ALA	2.3
1	C	716	ASP	2.3
1	D	166	ASP	2.3
1	D	319	LYS	2.3
1	A	570	ARG	2.3
1	C	490	THR	2.3
1	D	557	SER	2.3
1	D	410	PRO	2.3
1	D	650	PRO	2.3
1	D	689	GLY	2.3
1	D	715	GLY	2.3
1	C	665	ALA	2.2
1	D	39	ALA	2.2
1	C	563	LEU	2.2
1	D	382	LEU	2.2
1	C	589	LYS	2.2
1	C	594	LYS	2.2
1	D	523	LYS	2.2
1	D	598	LYS	2.2
1	A	716	ASP	2.2
1	C	200	ASP	2.2
1	C	396	ARG	2.2
1	D	147	ARG	2.2
1	A	676	SER	2.2
1	C	194	SER	2.2
1	D	466	VAL	2.2
1	C	678	GLY	2.2
1	B	635	PHE	2.2
1	C	98	GLU	2.2
1	C	585	ALA	2.2
1	D	253	LEU	2.2
1	D	378	GLU	2.2
1	D	619	ALA	2.2
1	B	584	LYS	2.2
1	B	671	LYS	2.2
1	D	270	LYS	2.2
1	D	662	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	542	GLN	2.2
1	D	89	GLN	2.2
1	D	483	ARG	2.2
1	C	195	VAL	2.2
1	D	165	THR	2.2
1	C	149	SER	2.2
1	B	630	GLY	2.2
1	C	61	GLY	2.2
1	C	286	GLY	2.2
1	D	180	PHE	2.2
1	A	682	LYS	2.2
1	D	273	LYS	2.2
1	D	274	ALA	2.2
1	D	489	LEU	2.2
1	D	288	ASN	2.2
1	D	404	GLN	2.2
1	D	595	ASP	2.2
1	B	541	PRO	2.2
1	B	625	VAL	2.2
1	C	97	PRO	2.2
1	C	400	PRO	2.2
1	C	568	THR	2.2
1	C	669	SER	2.2
1	D	149	SER	2.2
1	D	323	TYR	2.2
1	D	324	GLY	2.2
1	D	678	GLY	2.2
1	C	670	ALA	2.2
1	B	570	ARG	2.2
1	B	591	GLN	2.2
1	D	583	ASP	2.2
1	D	660	TRP	2.2
1	C	338	PHE	2.2
1	C	615	SER	2.2
1	D	693	GLU	2.2
1	D	461	ARG	2.1
1	D	612	GLN	2.1
1	C	254	VAL	2.1
1	D	343	VAL	2.1
1	B	716	ASP	2.1
1	C	55	MET	2.1
1	C	226	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	460	GLY	2.1
1	B	276	LEU	2.1
1	B	705	PHE	2.1
1	C	159	PHE	2.1
1	C	559	PHE	2.1
1	B	505	ALA	2.1
1	C	581	SER	2.1
1	C	47	GLU	2.1
1	C	167	GLU	2.1
1	C	649	ARG	2.1
1	D	346	GLU	2.1
1	D	504	GLU	2.1
1	D	649	ARG	2.1
1	D	498	ILE	2.1
1	B	350	ASN	2.1
1	D	550	ASN	2.1
1	D	243	MET	2.1
1	D	643	PRO	2.1
1	B	555	GLY	2.1
1	D	168	GLY	2.1
1	D	250	THR	2.1
1	B	674	LEU	2.1
1	D	344	LEU	2.1
1	C	631	ALA	2.1
1	C	658	TYR	2.1
1	D	603	ALA	2.1
1	A	642	SER	2.1
1	C	590	GLU	2.1
1	D	519	GLU	2.1
1	D	642	SER	2.1
1	B	638	LYS	2.1
1	C	169	ASN	2.1
1	C	287	LYS	2.1
1	D	231	MET	2.1
1	D	408	ASN	2.1
1	D	541	PRO	2.1
1	A	678	GLY	2.1
1	D	421	GLY	2.1
1	D	692	ASP	2.1
1	C	602	ILE	2.1
1	D	186	ILE	2.1
1	D	232	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	674	LEU	2.1
1	C	296	LEU	2.1
1	C	399	GLY	2.1
1	D	159	PHE	2.1
1	D	286	GLY	2.1
1	D	290	ASP	2.1
1	C	607	ALA	2.1
1	D	363	ILE	2.1
1	C	680	GLU	2.1
1	D	94	GLU	2.1
1	D	539	GLU	2.1
1	D	547	TYR	2.1
1	B	302	SER	2.0
1	D	428	HIS	2.0
1	A	559	PHE	2.0
1	C	707	PHE	2.0
1	D	711	PHE	2.0
1	C	553	THR	2.0
1	B	628	ALA	2.0
1	C	103	ALA	2.0
1	D	473	ALA	2.0
1	C	198	SER	2.0
1	C	608	SER	2.0
1	C	344	LEU	2.0
1	C	536	LEU	2.0
1	D	341	LEU	2.0
1	C	483	ARG	2.0
1	D	42	ARG	2.0
1	D	175	ASN	2.0
1	D	613	THR	2.0
1	C	301	GLU	2.0
1	D	50	ASP	2.0
1	A	571	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

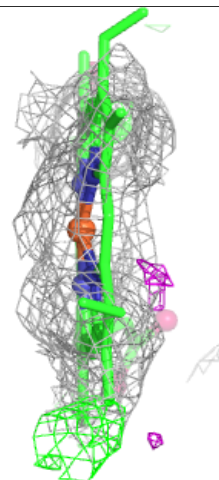
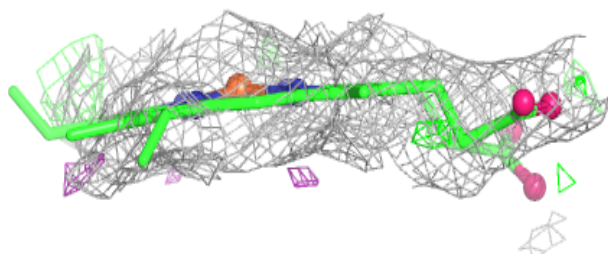
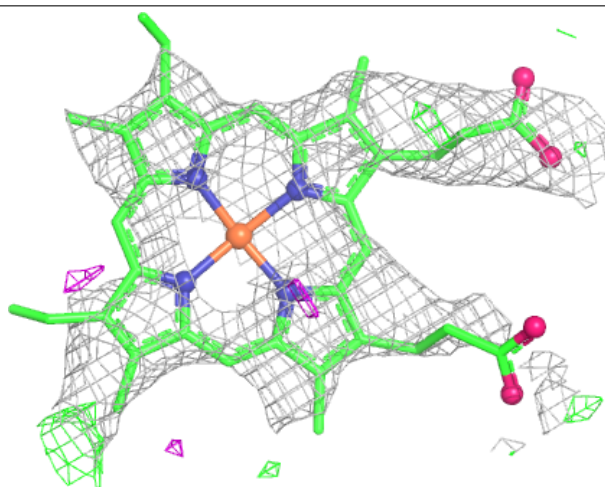
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	D	4000	43/43	0.73	0.21	92,93,97,101	0
2	HEM	C	4000	43/43	0.92	0.13	60,62,68,73	0
2	HEM	B	4000	43/43	0.93	0.11	43,46,50,59	0
2	HEM	A	4000	43/43	0.96	0.09	31,34,38,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

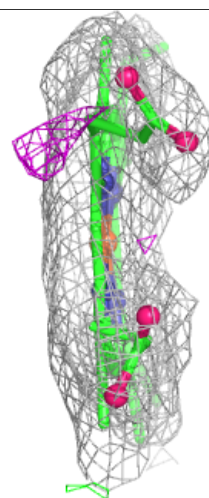
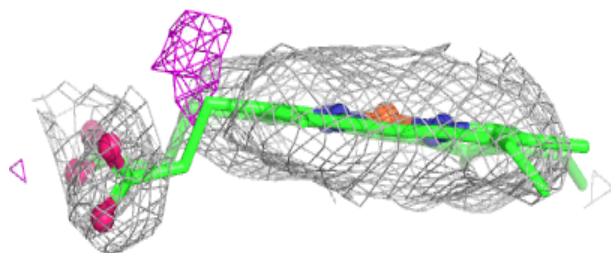
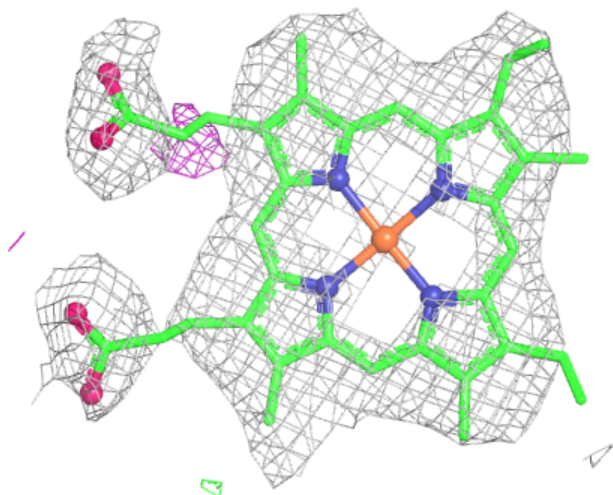
Electron density around HEM D 4000:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



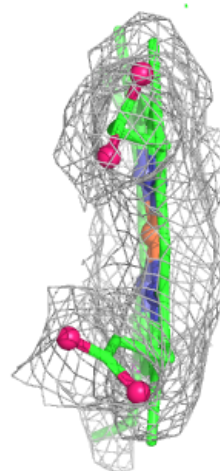
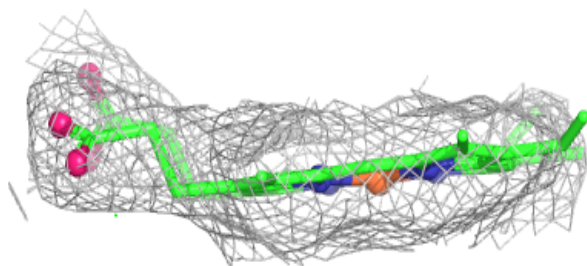
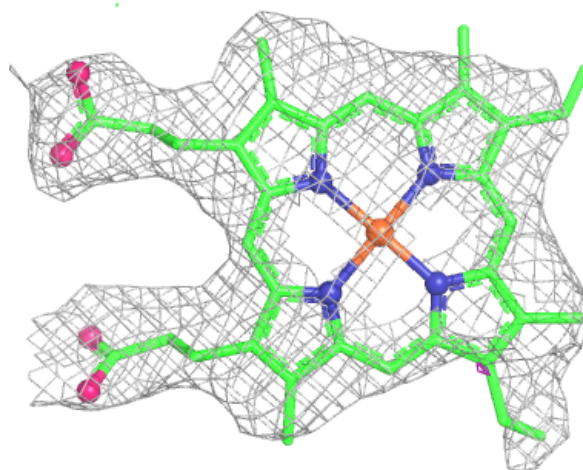
Electron density around HEM C 4000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



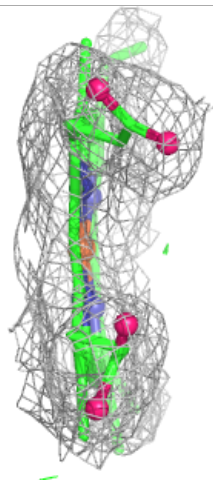
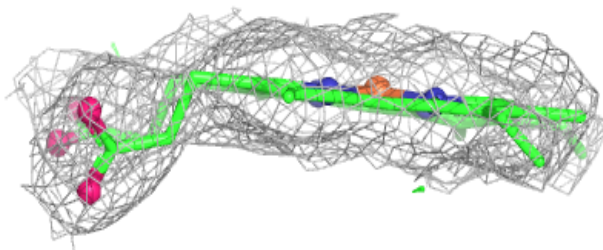
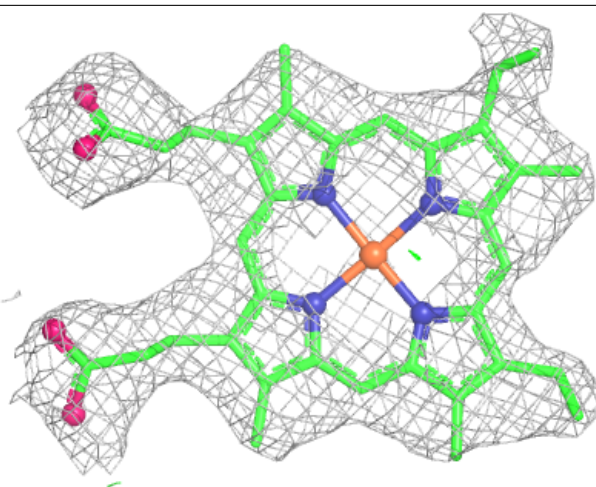
Electron density around HEM B 4000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 4000:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.